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US-6284154-\$.DID..USPT,JPAB,EPAB,DWPI,TDBD.	2
(US-6284154-\$.DID.).USPT,JPAB,EPAB,DWPI,TDBD.	2

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<u>L5</u>	us-6284154-\$.did.	2	<u>L5</u>
<u>L4</u>	jp-06184019-\$.did.	2	<u>L4</u>
<u>L3</u>	us-5474707-\$.did. or us-5536443-\$.did. or us-5653911-\$.did. or us-5645759-\$.did. or us-6056894-\$.did. or us-5382379-\$.did.	11	<u>L3</u>
<u>L2</u>	US-6319424-\$.did. or US-6270691-\$.did. or JP-11125825-\$.did. or JP-10068954-\$.did.	8	<u>L2</u>
<u>L1</u>	EP-1079244-\$.did.	2	<u>L1</u>

END OF SEARCH HISTORY

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L4: Entry 1 of 2

File: JPAB

Jul 5, 1994

PUB-NO: JP406184019A

DOCUMENT-IDENTIFIER: JP 06184019 A

TITLE: FLUOROALKYLCYCLOHEXANE DERIVATIVE

PUBN-DATE: July 5, 1994

INVENTOR-INFORMATION:

NAME

COUNTRY

TAKEHARA, SADAO

TAKATSU, HARUYOSHI

OGAWA, SHINJI

US-CL-CURRENT: 570/129

INT-CL (IPC): C07C 25/18; C09K 19/30; G02F 1/13

ABSTRACT:

PURPOSE: To obtain a new compound having low threshold voltage and high upper-limit temperature of liquid crystal phase to give a liquid crystal composition having broad temperature range of liquid crystal phase and low threshold voltage.

CONSTITUTION: The compound of formula I ((m) is 1 or 3; (n) is 0-5; Z1 and Z2 are single bond or CH2CH2 provided that at least one of Z" and Z2 is single bond; ring A is trans-1,4-cyclohexylene or 1,4-phenylene; X and Y are H or F; the cyclohexane ring has trans configuration), e.g. 3,4-difluoro-1-[trans-4-[trans-4-(2fluoroethyl)cyclohexyl]cyclohexyl]benzene. The compound can easily be produced by fluorinating a hydroxyalkylcyclohexane derivative of formula II with a fluorination agent such as diethylaminotrifluorosulfuric acid. The starting compound of formula II is easily producible from the corresponding cyclohexanone derivative of formula III. The compound of formula II wherein both X and Y are F is a new compound.

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 Derwent World Patents Index
 IBM Technical Disclosure Bulletins

Term:

us-5474707-\$.did. or us-5536443-\$.did. or
 us-5653911-\$.did. or us-5645759-\$.did. or
 us-6056894-\$.did. or us-5382379-\$.did.

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DB=USPT,JPAB,EPAB,DWPI,TDBD; PLUR=YES; OP=ADJ

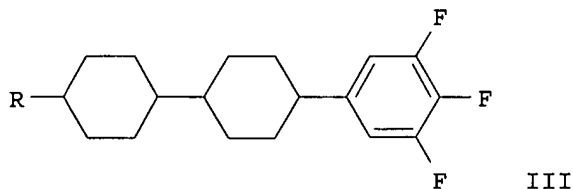
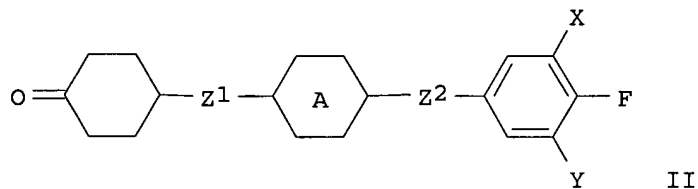
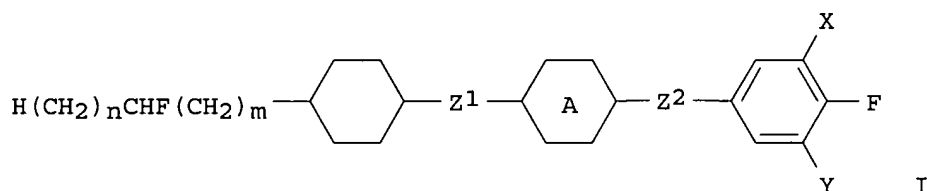
<u>L4</u>	jp-06184019-\$.did.	2	<u>L4</u>
<u>L3</u>	us-5474707-\$.did. or us-5536443-\$.did. or us-5653911-\$.did. or us-5645759-\$.did. or us-6056894-\$.did. or us-5382379-\$.did.	11	<u>L3</u>
<u>L2</u>	US-6319424-\$.did. or US-6270691-\$.did. or JP-11125825-\$.did. or JP-10068954-\$.did.	8	<u>L2</u>
<u>L1</u>	EP-1079244-\$.did.	2	<u>L1</u>

END OF SEARCH HISTORY

AN 1995:220392 CAPLUS
 DN 122:21003
 TI Preparation of (fluoroalkyl)cyclohexane derivatives as liquid crystals
 IN Takehara, Sadao; Takatsu, Haruyoshi; Ogawa, Shinji
 PA Dainippon Ink & Chemicals, Japan
 SO Jpn. Kokai Tokkyo Koho, 17 pp.
 CODEN: JKXXAF
 DT Patent
 LA Japanese
 IC ICM C07C025-18
 ICS C09K019-30; G02F001-13
 CC 75-11 (Crystallography and Liquid Crystals)
 Section cross-reference(s): 74
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 06184019	A2	19940705	JP 1993-139668	19930610
PRAI	JP 1992-150583		19920610		
	JP 1992-276342		19921014		
	JP 1992-286024		19921023		

GI



AB The title compds. (I; m = 1,3; n = 0-5; Z1, Z2 = single bond or CH2CH2, provided that at least one of Z1 and Z2 = single bond; ring A = trans-1,4-cyclohexylene or 1,4-phenylene; X, Y = H, F) are prepd. from intermediates, e.g. cyclohexanone derivs. (II; Z1, Z2, ring A = same as above). A liq. crystal compn. contains at least one I. (Fluoroalkyl)cyclohexane derivs. I show good compatibility with widely used nematic mother liq. crystals, excellent chem. stability and high specific resistance and voltage holding ratio owing to the absence of polar groups such as cyano and ester groups, and effect for lowering threshold voltage without lowering the temp. range of nematic phase when they are added to a liq. crystal compn., and thus can provide liq. crystal compns. showing nematic liq. crystal phase at wide temp. range up to high temp. and low threshold voltage and thereby useful for liq. crystal displays and particularly useful as active matrix-driving liq. crystal materials. Thus, Wittig reaction of cyclohexanone deriv. trans, trans-II

(Z1 = Z2 = single bond, ring A = 1,4-cyclohexylene) with MeOCH₂Ph₃PCl by using Me₃COK in THF and similar Wittig reaction of the resulting cyclohexanecarboxaldehyde deriv. (III; R = CHO) with MeOCH₂Ph₃PCl gave cyclohexylacetaldehyde deriv. III (R = OHCH₂) which was reduced by LiAlH₄ in THF to the alc. III (R = HOCH₂CH₂) and then fluorinated by DAST (Et₂NSF₃) in THF to give title compd. III (R = FCH₂CH₂) (IV). A liq. crystal compn. contg. 30 wt.% IV and an active-matrix mother liq. crystal (70 wt.%) consisting of 50% 4-[4-(4-vinylcyclohexyl)cyclohexyl]-1,2-difluorobenzene and 50% 4-[4-[4-(3-propen-1-yl)vinylcyclohexyl]cyclohexyl]-1,2-difluorobenzene showed the upper limit temp. of nematic phase at 98.6.degree. and threshold voltage (V_{th}) 2.00 V in a liq. crystal cell vs. 116.7.degree. and V_{th} = 2.43 V, resp., for the mother liq. crystal.

ST fluoroalkylcyclohexane deriv prepn liq crystal; active matrix nematic liq crystal display

IT Liquid crystals
(prepn. of (fluoroalkyl)cyclohexane derivs. as liq. crystals)

IT Optical imaging devices
(electrooptical liq.-crystal, prepn. of (fluoroalkyl)cyclohexane derivs. as liq. crystals for (active matrix) nematic liq. crystal displays)

IT 56309-94-5
RL: RCT (Reactant)
(Grignard addn. with bromotrifluorobenzene in prepn. of (fluoroalkyl)cyclohexane derivs. as liq. crystals)

IT 138526-69-9, 1-Bromo-3,4,5-trifluorobenzene
RL: RCT (Reactant)
(Grignard addn. with cyclohexanone deriv. in prepn. of (fluoroalkyl)cyclohexane derivs. as liq. crystals)

IT 4009-98-7, Methoxymethyltriphenylphosphonium chloride
RL: RCT (Reactant)
(Wittig reaction with formylcyclohexane deriv. in prepn. of (fluoroalkyl)cyclohexane derivs. as liq. crystals)

IT 145767-92-6 159386-26-2
RL: RCT (Reactant)
(Wittig reaction with methoxymethyltriphenylphosphonium chloride in prepn. of (fluoroalkyl)cyclohexane derivs. as liq. crystals)

IT 75-16-1, Methylmagnesium bromide
RL: RCT (Reactant)
(addn. reaction with hexylacetaldehyde deriv. in prepn. of (fluoroalkyl)cyclohexane derivs. as liq. crystals)

IT 155266-68-5
RL: RCT (Reactant)
(hydroboration-oxidative hydroxylation in prepn. of (fluoroalkyl)cyclohexane derivs. as liq. crystals)

IT 159386-27-3P 159386-28-4P 159386-29-5P 159386-30-8P 159386-31-9P
159386-32-0P 159386-33-1P 159386-34-2P 159386-35-3P 159386-36-4P
159386-37-5P 159386-38-6P 159386-39-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(intermediate for prepn. of (fluoroalkyl)cyclohexane derivs. as liq. crystals)

IT 159516-04-8 159516-05-9
RL: DEV (Device component use); USES (Uses)
(nematic liq. crystal compn. for active-matrix liq. crystal displays)

IT 61203-99-4 61204-01-1 61204-03-3 67589-39-3 67589-41-7
67589-46-2 67589-47-3 67589-52-0 67589-53-1
RL: DEV (Device component use); USES (Uses)
(nematic liq. crystal compn. for liq. crystal displays)

IT 159386-20-6P 159386-21-7P 159386-22-8P 159386-23-9P 159386-24-0P
159386-25-1P
RL: DEV (Device component use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(prepn. of (fluoroalkyl)cyclohexane derivs. as liq. crystals for (active matrix) nematic liq. crystal displays)

IT 159516-04-8

RL: DEV (Device component use); USES (Uses)

(nematic liq. crystal compn. for active-matrix liq. crystal displays)

RN 159516-04-8 CAPLUS

CN Benzene, 4-[4'-(3-butenyl)[1,1'-bicyclohexyl]-4-yl]-1,2-difluoro-,
[trans(trans)]-, mixt. with [trans(trans)]-1,2-difluoro-4-[4'-(2-
fluorobutyl)[1,1'-bicyclohexyl]-4-yl]benzene and [trans(trans)]-4-(4'-
ethenyl[1,1'-bicyclohexyl]-4-yl)-1,2-difluorobenzene (9CI) (CA INDEX
NAME)

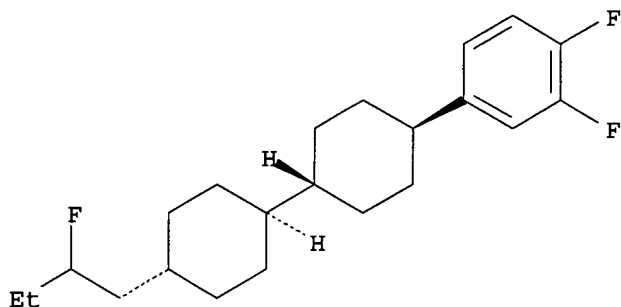
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CRN 159386-24-0

CMF C22 H31 F3

CDES *

Relative stereochemistry.



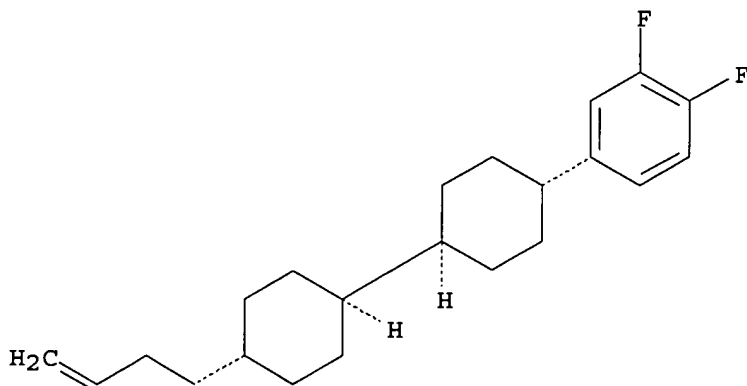
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CRN 155266-68-5

CMF C22 H30 F2

CDES *

Relative stereochemistry.



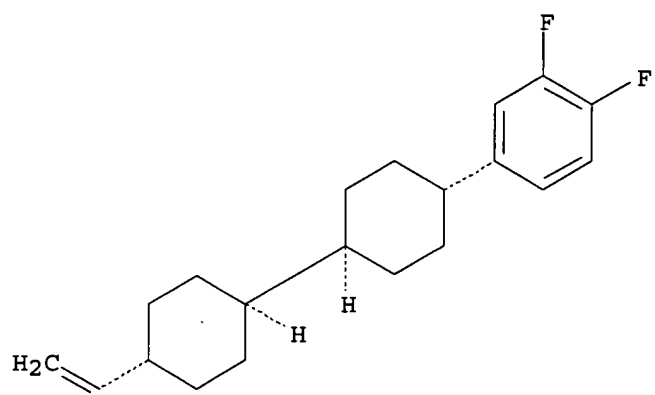
CM 3

CRN 142400-92-8

CMF C20 H26 F2

CDES *

Relative stereochemistry.



AN 1995:861146 CAPLUS
 DN 123:301635
 TI Cyclic hydrocarbon derivative and liquid crystal composition containing the same.
 IN Takatsu, Haruyoshi; Takehara, Sadao; Takeuchi, Kiyohumi; Osawa, Masashi; Ogawa, Shinji; Ishida, Norie
 PA Dainippon Ink Chemical Industry Co., Japan
 SO Eur. Pat. Appl., 334 pp.
 CODEN: EPXXDW
 DT Patent
 LA English
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 637623	A1	19950208	EP 1994-111448	19940722
	EP 637623	B1	20011004		
	R: DE, GB				
	JP 07034066	A2	19950203	JP 1993-182734	19930723
	US 5474707	A	19951212	US 1994-278260	19940721
	US 5536443	A	19960716	US 1995-429485	19950425
PRAI	JP 1993-182734	A	19930723		
	US 1994-278260	A3	19940721		
OS	MARPAT 123:301635				

1, 4-5, 7-8

6

3

AN 1995:995628 CAPLUS
 DN 124:131646
 TI Liquid crystalline compound, liquid crystal composition, and display element.
 IN Kondo, Tomoyuki; Miyazawa, Kazutoshi; Fujita, Atsuko; Ohnishi, Noriyuki; Goto, Yasuyuki; Nakagawa, Etsuo; Sawada, Shinichi
 PA Chisso Corp., Japan
 SO Eur. Pat. Appl., 66 pp.
 CODEN: EPXXDW
 DT Patent
 LA English
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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PI	EP 679707	A1	19951102	EP 1995-302894	19950428
	EP 679707	B1	19990616		
	R: AT, CH, DE, FR, GB, IT, LI, NL				
	JP 08012605	A2	19960116	JP 1995-64200	19950323
	US 5653911	A	19970805	US 1995-429847	19950427
	CN 1117515	A	19960228	CN 1995-104596	19950428
	AT 181352	E	19990715	AT 1995-302894	19950428
	US 5720899	A	19980224	US 1996-775199	19961230
PRAI	JP 1994-92740		19940428		
	US 1995-429847		19950427		
OS	MARPAT 124:131646				

AN 1996:304000 CAPLUS
 DN 124:356419
 TI A liquid crystal composition and a liquid crystal display element using
 the same
 IN Tomi, Yoshitaka; Nakagawa, Etsuo; Sawada, Shinichi
 PA Chisso Corp., Japan
 SO Eur. Pat. Appl., 34 pp.
 CODEN: EPXXDW

DT Patent
 LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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PI	EP 704512	A1	19960403	EP 1995-113991	19950906
	EP 704512	B1	20000308		
	R: CH, DE, GB, LI				
	JP 08073857	A2	19960319	JP 1994-238555	19940906
	US 5645759	A	19970708	US 1995-524441	19950906
PRAI	JP 1994-238555		19940906		
OS	MARPAT 124:356419				

AN 1998:589506 CAPLUS
 DN 129:223330
 TI TN- and STN-liquid crystal display with fast switching time
 IN Hirschmann, Harald; Reiffenrath, Volker; Weller, Clarissa
 PA Merck Patent G.m.b.H., Germany
 SO Ger. Offen., 46 pp.
 CODEN: GWXXBX

DT Patent
 LA German

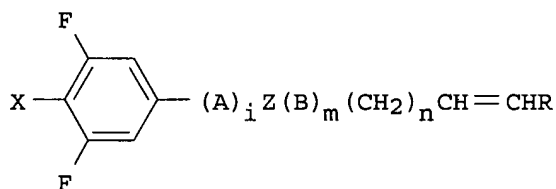
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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PI	DE 19707956	A1	19980903	DE 1997-19707956	19970227
	GB 2322631	A1	19980902	GB 1998-4136	19980226
	GB 2322631	B2	20010221		
	CN 1192464	A	19980909	CN 1998-105339	19980226
	US 6056894	A	20000502	US 1998-30921	19980226
	JP 10245560	A2	19980914	JP 1998-62030	19980227
PRAI	DE 1997-19707956	A	19970227		
OS	MARPAT 129:223330				

AN 1995:252460 CAPLUS
 DN 122:148170
 TI Preparation of cyclohexane derivatives as liquid crystals
 IN Onchi, Juichi; Shioda, Makoto; Matsui, Shuichi; Kondo, Tomoyuki; Goto, Yasuyuki
 PA Chisso Corp, Japan
 SO Jpn. Kokai Tokkyo Koho, 57 pp.
 CODEN: JKXXAF
 DT Patent
 LA Japanese
 IC ICM C07C025-18
 ICS C07C043-225; C09K019-30
 CC 75-11 (Crystallography and Liquid Crystals)
 Section cross-reference(s): 74

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 06211711	A2	19940802	JP 1993-250740	19931006
	JP 2908968	B2	19990623		
	US 5382379	A	19950117	US 1993-132917	19931007
PRAI	JP 1992-268868		19921007		
OS	MARPAT 122:148170				
GI					



AB The title compds. [I; R = H, trans-C1-7 linear or branched alkyl; X = F, CF3, CF3O, F2CH; A = 1,4-cyclohexylene, 1,4-phenylene; B = 1,4-cyclohexylene; i, m = 0,1,2; (i + m).gtoreq.1; Z = single bond, CH2CH2; n = 0-4] are prepd. A liq. crystal compn. contains at least one I. These cyclohexane derivs. I have low viscosity and unexpectedly lower elastic const. ratio (K33/K11) than those of compds. having n-alkyl substituents in spite of the presence of the alkenyl substituent, decrease thresh-hold voltage of display devices when they are added to a liq. crystal compn., and are suitable for the use in twisted nematic (TN)-mode liq. crystal display devices. Thus, treatment of EtPh3PBr with Me3COK in THF at 0.degree. followed by Wittig reaction with 3-[4-(3,4,5-trifluorophenyl)cyclohexyl]propionaldehyde at room temp. gave 5-[4-(3,4,5-trifluorophenyl)cyclohexyl]-2-pentene (II) which was converted into (2E)-II by epoxidn. of II with m-chloroperbenzoic acid in CH2Cl2, bromination of the resulting epoxide with Ph3PBr2 in refluxing benzene, and debromination of the resulting 2,3-dibromopentane deriv. with Zn powder in AcOH. A liq. crystal compn. contg. 15 wt.% (2E)-II and a mixt. of 5 p-cyclohexylbenzonitrile derivs. (85 wt.%) showed the nematic-isotropic phase transition at -95.6.degree., viscosity 2.3 cp at 20.degree., and threshold voltage 1.28 V and elastic const. ratio K33/K11 = 1.99 in a TN liq. crystal cell.

ST cyclohexane deriv prepn liq crystal; twisted nematic liq crystal display device

IT Liquid crystals
 (prepn. of cyclohexane derivs. as liq. crystals)

IT Optical imaging devices
 (electrooptical liq.-crystal, prepn. of cyclohexane derivs. as liq. crystals for twisted nematic liq. crystal display)

IT 138526-69-9 156243-64-0, 3,5-Difluoro-4-trifluoromethylbromobenzene

RL: RCT (Reactant)
 (Grignard addn. with cyclohexanone deriv. in prepn. of cyclohexane
 derivs. as liq. crystals)

IT 4746-97-8, 1,4-Cyclohexanedione monoethylene ketal 56309-94-5,
 4,4'-Dicyclohexanedione monoethylene ketal 160910-66-7,
 1,1-Ethylenedioxy-4-[2-(4-oxocyclohexyl)ethyl]cyclohexanone
 RL: RCT (Reactant)
 (Grignard addn. with trifluorobromobenzene in prepn. of cyclohexane
 derivs. as liq. crystals)

IT 867-13-0, Triethyl phosphonoacetate
 RL: RCT (Reactant)
 (Horner-Emmons reaction with cyclohexanone deriv. in prepn. of
 cyclohexane derivs. as liq. crystals)

IT 2043-61-0, Formylcyclohexane 160910-65-6
 RL: RCT (Reactant)
 (Wittig reaction with benzyltriphenylphosphonium bromide deriv. in
 prepn. of cyclohexane derivs. as liq. crystals)

IT 1779-49-3, Methyltriphenylphosphonium bromide
 RL: RCT (Reactant)
 (Wittig reaction with cyclohexanecarboxaldehyde deriv. in prepn. of
 cyclohexane derivs. as liq. crystals)

IT 4009-98-7, Methoxymethyltriphenylphosphonium chloride 69891-92-5,
 2-(1,3-Dioxan-2-yl)ethyltriphenylphosphonium bromide
 RL: RCT (Reactant)
 (Wittig reaction with cyclohexanone deriv. in prepn. of cyclohexane
 derivs. as liq. crystals)

IT 1530-32-1, Ethyltriphenylphosphonium bromide
 RL: RCT (Reactant)
 (Wittig reaction with cyclohexylpropionaldehyde deriv. in prepn. of
 cyclohexane derivs. as liq. crystals)

IT 160910-64-5, 3,4,5-Trifluorobenzyltriphenylphosphonium bromide
 RL: RCT (Reactant)
 (Wittig reaction with formylcyclohexane in prepn. of cyclohexane
 derivs. as liq. crystals)

IT 152816-09-6P 159386-29-5P 159386-30-8P 159386-31-9P 159386-32-0P
 159386-39-7P 160148-04-9P 160148-05-0P 160148-06-1P 160148-08-3P
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 160910-33-8P 160910-34-9P 160910-35-0P 160910-36-1P 160910-37-2P
 160910-38-3P 160910-39-4P 160910-40-7P 160910-41-8P 160910-42-9P
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 160910-58-7P 160910-59-8P 160910-60-1P 160910-61-2P 160910-62-3P
 160910-63-4P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
 (intermediate for prepn. of cyclohexane derivs. as liq. crystals for
 twisted nematic liq. crystal display)

IT 160910-23-6 160910-24-7 161022-29-3 161022-30-6
 161022-31-7
 RL: DEV (Device component use); USES (Uses)
 (liq. crystal compn. for twisted nematic liq. crystal display)

IT 160910-14-5P
 RL: DEV (Device component use); RCT (Reactant); SPN (Synthetic
 preparation); PREP (Preparation); USES (Uses)
 (prepn. of cyclohexane derivs. as liq. crystals for twisted nematic
 liq. crystal display)

IT 159586-97-7P 160910-15-6P 160910-16-7P 160910-17-8P 160910-18-9P
 160910-19-0P 160910-20-3P 160910-21-4P 160910-22-5P
 RL: DEV (Device component use); SPN (Synthetic preparation); PREP
 (Preparation); USES (Uses)
 (prepn. of cyclohexane derivs. as liq. crystals for twisted nematic
 liq. crystal display)

IT 161022-29-3

RL: DEV (Device component use); USES (Uses)

(liq. crystal compn. for twisted nematic liq. crystal display)

RN 161022-29-3 CAPLUS

CN Benzonitrile, 4-(4-heptylcyclohexyl)-, trans-, mixt. with
[trans(trans)]-4-(4'-pentyl[1,1'-bicyclohexyl]-4-yl)benzonitrile,
trans-4-(4-pentylcyclohexyl)benzonitrile, trans-4-(4-
propylcyclohexyl)benzonitrile and [1.alpha.,4.beta.(E)]-1,2,3-trifluoro-5-
[4-(3-pentenyl)cyclohexyl]benzene (9CI) (CA INDEX NAME)

CM 1

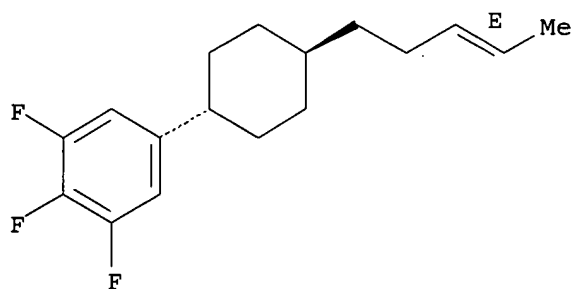
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CMF C17 H21 F3

CDES *

Relative stereochemistry.

Double bond geometry as shown.



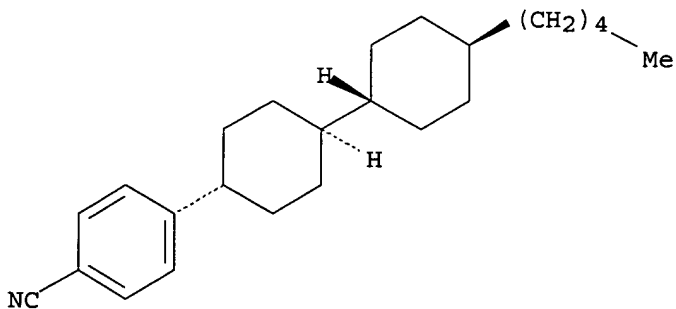
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CRN 85547-03-1

CMF C24 H35 N

CDES *

Relative stereochemistry.



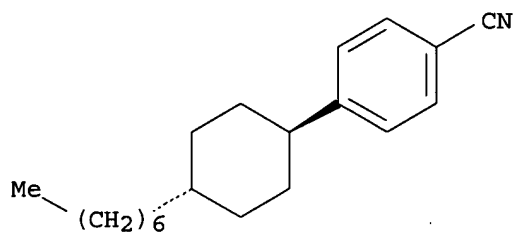
CM 3

CRN 61204-03-3

CMF C20 H29 N

CDES 2:TRANS

Relative stereochemistry.



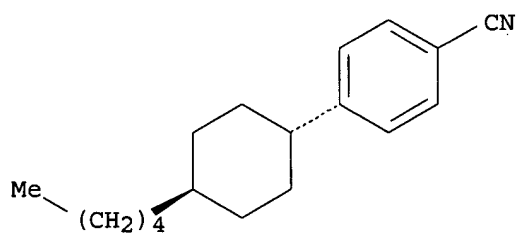
CM 4

CRN 61204-01-1

CMF C18 H25 N

CDES 2:TRANS

Relative stereochemistry.



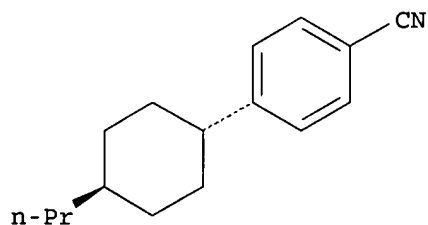
CM 5

CRN 61203-99-4

CMF C16 H21 N

CDES 2:TRANS

Relative stereochemistry.



IT 160910-21-4P

RL: DEV (Device component use); SPN (Synthetic preparation); PREP

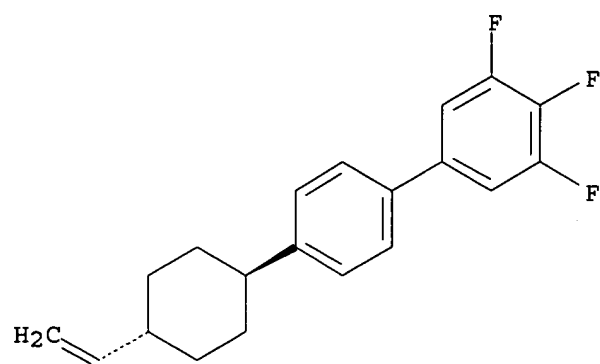
(Preparation); USES (Uses)

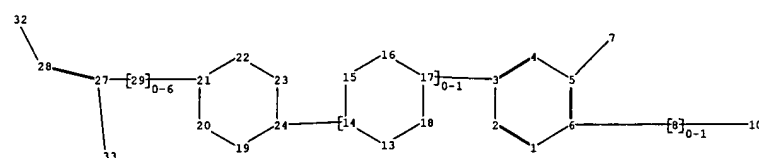
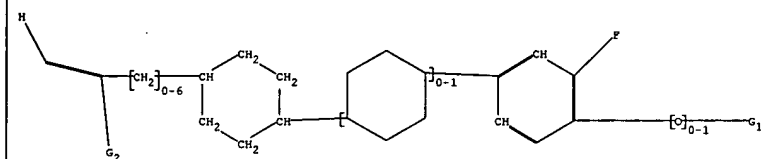
(prepn. of cyclohexane derivs. as liq. crystals for twisted nematic liq. crystal display)

RN 160910-21-4 CAPLUS

CN 1,1'-Biphenyl, 4'-(trans-4-ethenylcyclohexyl)-3,4,5-trifluoro- (9CI) (CA INDEX NAME)

Relative stereochemistry.





chain nodes :

7 8 10 27 28 29 32 33

ring nodes :

1 2 3 4 5 6 13 14 15 16 17 18 19 20 21 22 23 24

chain bonds :

3-17 5-7 6-8 8-10 14-24 21-29 27-28 27-29 27-33 28-32

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 13-14 13-18 14-15 15-16 16-17 17-18 19-20 19-24
20-21 21-22 22-23 23-24

exact/norm bonds :

6-8 8-10 13-14 13-18 14-15 15-16 16-17 17-18 19-20 19-24 20-21 21-22 22-23
23-24 27-33

exact bonds :

3-17 5-7 14-24 21-29 27-28 27-29 28-32

normalized bonds :

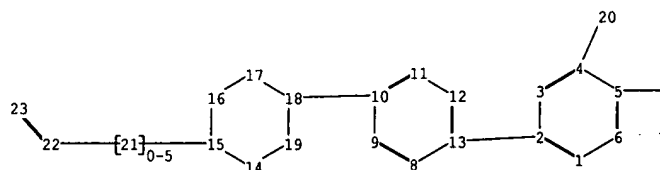
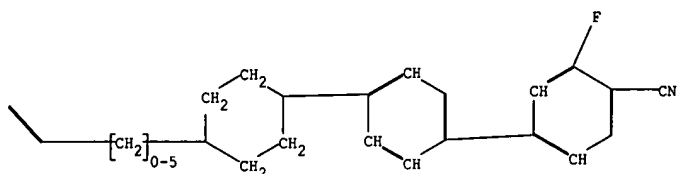
1-2 1-6 2-3 3-4 4-5 5-6

G1:Cl,F,CF2,CF3

G2:H,CH3

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 10:CLASS 13:Atom
14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom 23:Atom
24:Atom 27:CLASS 28:CLASS 29:CLASS 32:CLASS 33:CLASS



chain nodes :

7 20 21 22 23

ring nodes :

1 2 3 4 5 6 8 9 10 11 12 13 14 15 16 17 18 19

chain bonds :

2-13 4-20 5-7 10-18 15-21 21-22 22-23

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 8-9 8-13 9-10 10-11 11-12 12-13 14-15 14-19 15-16
16-17 17-18 18-19

exact/norm bonds :

14-15 14-19 15-16 16-17 17-18 18-19

exact bonds :

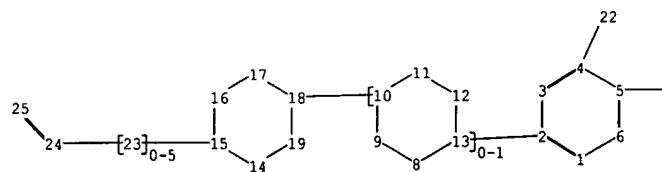
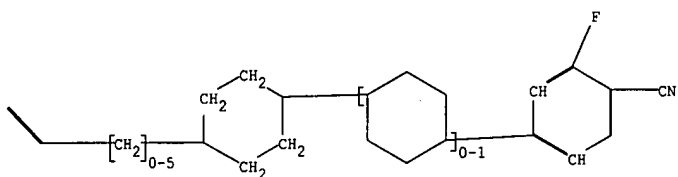
2-13 4-20 5-7 10-18 15-21 21-22 22-23

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 8-9 8-13 9-10 10-11 11-12 12-13

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:CLASS
21:CLASS 22:CLASS 23:CLASS



chain nodes :

7 22 23 24 25

ring nodes :

1 2 3 4 5 6 8 9 10 11 12 13 14 15 16 17 18 19

chain bonds :

2-13 4-22 5-7 10-18 15-23 23-24 24-25

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 8-9 8-13 9-10 10-11 11-12 12-13 14-15 14-19 15-16
16-17 17-18 18-19

exact/norm bonds :

8-9 8-13 9-10 10-11 11-12 12-13 14-15 14-19 15-16 16-17 17-18 18-19

exact bonds :

2-13 4-22 5-7 10-18 15-23 23-24 24-25

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

Match level :

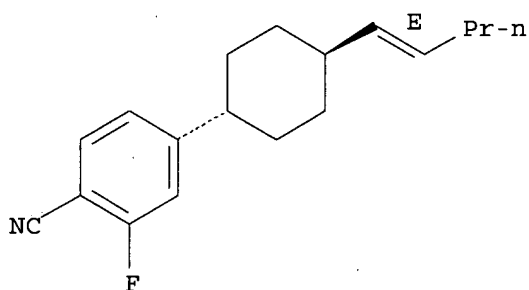
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 22:CLASS
23:CLASS 24:CLASS 25:CLASS

RN 105942-13-0 REGISTRY
 CN Benzonitrile, 2-fluoro-4-[4-(1-pentenyl)cyclohexyl]-,
 [1.alpha.,4.beta.(E)]- (9CI) (CA INDEX NAME)
 FS STEREOSEARCH
 MF C18 H22 F N
 SR CA
 LC STN Files: CA, CAPLUS, USPATFULL

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C6	C6	6	C6	46.150.1	1
C6	C6	6	C6	46.150.18	1

Relative stereochemistry.
 Double bond geometry as shown.



$r = 0$
 $Q' \neq Q'' = H$
 $n = 3$
 $A = \text{single}$
 $X = CN$
 $Y \text{ or } Z = F$

Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	27799	pH 1	(1) ACD
Bioconc. Factor (BCF)	27799	pH 4	(1) ACD
Bioconc. Factor (BCF)	27799	pH 7	(1) ACD
Bioconc. Factor (BCF)	27799	pH 8	(1) ACD
Bioconc. Factor (BCF)	27799	pH 10	(1) ACD
Boiling Point (BP)	373.0+/-27.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	62.02+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	194.7+/-25.2 deg C		(1) ACD
Freely Rotatable Bonds (FRB)	4		(1) ACD
H acceptors (HAC)	1		(1) ACD
H donors (HD)	0		(1) ACD
Koc (KOC)	52798	pH 1	(1) ACD
Koc (KOC)	52798	pH 4	(1) ACD
Koc (KOC)	52798	pH 7	(1) ACD
Koc (KOC)	52798	pH 8	(1) ACD
Koc (KOC)	52798	pH 10	(1) ACD
logD (LOGD)	6.15	pH 1	(1) ACD
logD (LOGD)	6.15	pH 4	(1) ACD
logD (LOGD)	6.15	pH 7	(1) ACD
logD (LOGD)	6.15	pH 8	(1) ACD
logD (LOGD)	6.15	pH 10	(1) ACD
logP (LOGP)	6.150+/-0.361		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD

Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	271.37		(1) ACD
Vapor Pressure (VP)	9.24E-06 Torr	25.0 deg C	(1) ACD

(1) Calculated using Advanced Chemistry Development (ACD) Software Solaris V4.76 ((C) 1994-2003 ACD)

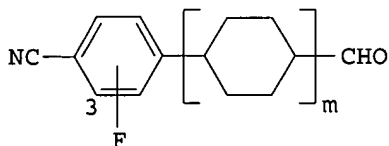
1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1

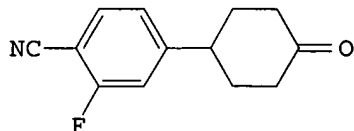
AN 106:18142 CA
TI Fluorobenzonitrile derivatives as intermediates for liquid crystal materials
IN Waechtler, Andreas; Kurmeier, Hans Adolf; Hittich, Reinhard; Scheuble, Bernhard
PA Merck Patent G.m.b.H., Fed. Rep. Ger.
SO Ger. Offen., 22 pp.
CODEN: GWXXBX
DT Patent
LA German
IC ICM C07C121-76
ICS C07C120-00; C09K019-08
CC 25-20 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 75

FAN.CNT 1

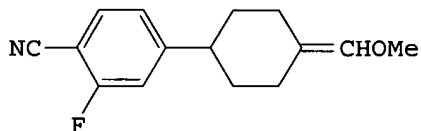
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 3504866	A1	19860814	DE 1985-3504866	19850213
	WO 8604895	A1	19860828	WO 1986-EP40	19860130
	W: JP, US				
	RW: AT, BE, CH, DE, FR, GB, IT, LU, NL, SE				
	EP 211876	A1	19870304	EP 1986-901063	19860130
	R: CH, DE, GB, LI				
	JP 62501842	T2	19870723	JP 1986-500899	19860130
	<u>US 4784471</u>	A	19881115	US 1986-932544	19861014
PRAI	DE 1985-3504866		19850213		
	WO 1986-EP40		19860130		
GI					



I



II



III

AB The title compds. I ($m = 0, 1$) are prepd. as intermediates for liq. crystal materials. Thus, a suspension of 5.3 g $\text{Ph}_3(\text{MeOCH}_2)\text{P}^+\text{Cl}^-$ and 1.8 g KOCMe_3 in diisopropyl ether was treated with 2.3 g (cyanofluorophenyl)cyclohexanone II in THF at -15°C , and the resulting methoxymethylene deriv. III was acidified to give trans-I

(3-fluoro; m = 1), which was treated with HOCH₂CH(Pr)CH₂OH in PhMe in the presence of p-toluenesulfonic acid to give the liq. crystal material

ST 2-[trans-4-(4-cyano-3-fluorophenyl)cyclohexyl]-5-propyl-1,3-dioxane.
fluorobenzonitrile prepn liq crystal intermediate

IT Liquid crystals
(intermediates for, fluorobenzonitrile derivs. as)

IT 105942-12-9, 4-(3-Fluoro-4-cyanophenyl)cyclohexanecarboxaldehyde
RL: RCT (Reactant); RACT (Reactant or reagent)
(Wittig reaction of, liq. crystal material from)

IT 1779-51-7, n-Butyltriphenylphosphonium bromide
RL: RCT (Reactant); RACT (Reactant or reagent)
(Wittig reaction of, with cyclohexanecarboxaldehyde deriv.)

IT 23523-33-3, Bis(triphenylphosphine)palladium dibromide
RL: CAT (Catalyst use); USES (Uses)
(catalyst, for formylation of bromofluorobenzonitrile)

IT 105942-08-3, 4-Bromo-2-fluorobenzonitrile
RL: RCT (Reactant); RACT (Reactant or reagent)
(formylation of)

IT 105942-09-4, 2-Fluoro-4-cyanobenzyl bromide
RL: RCT (Reactant); RACT (Reactant or reagent)
(oxidn. of)

IT 105942-11-8, 4,4'-Dicyano-3,3'-difluorostilbene
RL: RCT (Reactant); RACT (Reactant or reagent)
(ozonolysis of)

IT 105942-07-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and Wittig reaction of, as intermediate for liq. crystal materials)

IT 105942-06-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and hydrolysis of)

IT 105942-13-0P 105942-14-1P 105942-16-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

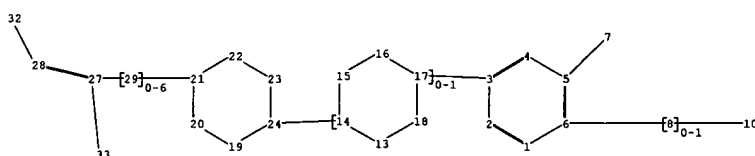
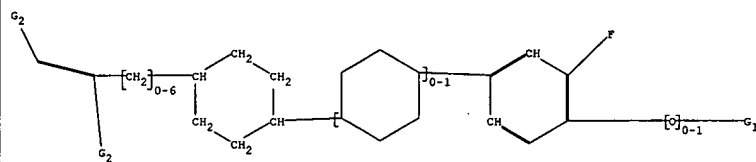
IT 101048-76-4P, 3-Fluoro-4-cyanobenzaldehyde 105942-10-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, as intermediate for liq. crystal materials)

IT 4009-98-7, Triphenylmethoxymethylphosphonium chloride
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with (cyanofluorophenyl)cyclohexanone)

IT 2612-28-4, 2-Propylpropane-1,3-diol
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with aldehyde, liq. crystal materials from)

IT 105942-15-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with propylpropanediol, liq. crystal material from)

IT 105942-05-0, 4-(4-Cyano-3-fluorophenyl)cyclohexanone
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with triphenyl(methoxymethyl)phosphonium chloride)



chain nodes :

7 8 10 27 28 29 32 33

ring nodes :

1 2 3 4 5 6 13 14 15 16 17 18 19 20 21 22 23 24

chain bonds :

3-17 5-7 6-8 8-10 14-24 21-29 27-28 27-29 27-33 28-32

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 13-14 13-18 14-15 15-16 16-17 17-18 19-20 19-24
20-21 21-22 22-23 23-24

exact/norm bonds :

6-8 8-10 13-14 13-18 14-15 15-16 16-17 17-18 19-20 19-24 20-21 21-22 22-23
23-24 27-33 28-32

exact bonds :

3-17 5-7 14-24 21-29 27-28 27-29

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

G1:Cl,F,CF2,CF3,CN

G2:H,CH3

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 10:CLASS 13:Atom
14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom 23:Atom
24:Atom 27:CLASS 28:CLASS 29:CLASS 32:CLASS 33:CLASS

AN 1995:861146 CAPLUS
 DN 123:301635
 TI Cyclic hydrocarbon derivative and liquid crystal composition containing the same.
 IN Takatsu, Haruyoshi; Takehara, Sadao; Takeuchi, Kiyohumi; Osawa, Masashi; Ogawa, Shinji; Ishida, Norie
 PA Dainippon Ink Chemical Industry Co., Japan
 SO Eur. Pat. Appl., 334 pp.
 CODEN: EPXXDW
 DT Patent
 LA English
 IC ICM C09K019-04
 ICS C09K019-30; C07B059-00; C07C255-50; C07C043-20; C07C025-18
 CC 74-13 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)
 Section cross-reference(s): 75

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 637623	A1	19950208	EP 1994-111448	19940722
	EP 637623	B1	20011004		
	R: DE, GB				
	JP 07034066	A2	19950203	JP 1993-182734	19930723
	US 5474707	A	19951212	US 1994-278260	19940721
	US 5536443	A	19960716	US 1995-429485	19950425
PRAI	JP 1993-182734	A	19930723		
	US 1994-278260	A3	19940721		
OS	MARPAT 123:301635				
GI					

1, 7, 8

9, 10, 12, 13

14, 15

18, 19, 20, 21

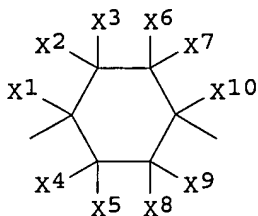
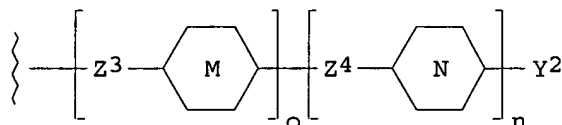
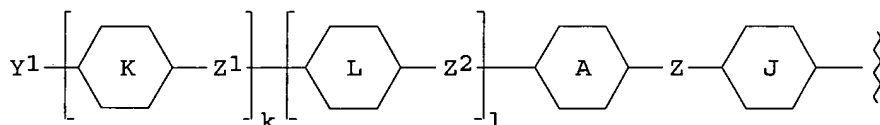
22-29, 30-31

I 32-35

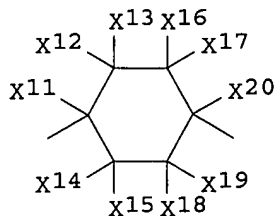
36-38, 39

40-47

50-53, 48-49



II



III

AB A novel cyclic hydrocarbon deriv. is disclosed, which is represented by formula I, wherein Y1 and Y2 each independently represent F, Cl, CN, OCN, SCN, OCF3, OCF2H, OCH2CF3, CF3, R, OR, CO2R, or -OCOR, wherein R represents alkyl having 1-20 C atoms, alkenyl having from 2-20 C atoms, or alkoxyalkyl having 2-20 C atoms, provided that at least one of Y1 and Y2 represents R, OR, CO2R, or -OCOR; Z, Z1-4 each independently represent a single bond, CH2CH2, CH=CH, C.tplbond.C, CO2, OCO, CH2O, OCH2, (CH2)4, (CH2)30, or O(CH2)3; ring A represents a group of formula II, wherein

X1-10 each independently represent H or D, provided that at least one of them represents D; rings K, L, J, M, N each independently represent trans-1,4-cyclohexylene, 1,4-cyclohexenylene, trans-1,4-phenylene, 1,4-phenylene substituted with 1-4 substituents selected from F, Cl, CN, and CH₃, 1,3-dioxane-2,6-diyl, pyrimidine-2,5-diyl, pyridine-2,5-diyl, or a group of formula III, wherein X11-20 each independently represent H or D, provided that at least one of them represents D; k, l, m, n each independently represent 0 or 1 with the sum of k, l, m, and n being 0, 1, or 2 is prep'd. and used in a liq. crystal compn. for an electrooptical display device.

ST cyclic hydrocarbon liq crystal display

IT Liquid crystals

(cyclic hydrocarbons as)

IT Optical imaging devices

(electrooptical, liq. crystal compns. contg. cyclic hydrocarbons for)

IT 169273-07-8 169273-17-0 169273-19-2 169273-20-5 169273-21-6
169527-81-5 169527-83-7 169527-84-8 169527-85-9 169527-86-0
169527-87-1 169527-88-2 169527-89-3 169527-90-6 169527-91-7
169532-92-7

RL: TEM (Technical or engineered material use); USES (Uses)

(display device liq. crystal compn.)

IT 61203-99-4 61204-01-1 61204-03-3 67589-39-3 67589-41-7
67589-46-2 67589-47-3 67589-52-0 67589-53-1 86504-59-8
92118-81-5 92118-82-6 92118-83-7 92118-84-8 93743-04-5
94819-16-6 94840-77-4 96042-33-0 97941-21-4 119990-81-7
129738-54-1 142400-92-8 144916-76-7 147065-76-7 155041-85-3
155266-68-5 159586-97-7 162785-84-4 162785-85-5 163671-84-9
163671-92-9 163671-97-4 167949-21-5 167949-22-6 167949-24-8
167949-26-0 167949-27-1 169151-78-4 169151-79-5 169151-80-8
169151-81-9 169151-82-0 169151-83-1 169151-84-2 169151-85-3
169151-86-4 169151-87-5 169151-88-6 169151-89-7 169151-90-0
169151-91-1 169151-92-2 169151-93-3 169151-94-4 169151-95-5
169151-96-6 169151-97-7 169151-98-8 169151-99-9 169152-00-5
169152-01-6 169152-02-7 169152-03-8 169152-04-9 169152-05-0
169152-06-1 169152-07-2 169152-08-3 169152-09-4 169152-10-7
169152-11-8 169152-12-9 169152-13-0 169152-14-1 169152-15-2
169152-16-3 169152-17-4 169152-18-5 169152-19-6 169152-20-9
169152-21-0 169152-22-1 169152-23-2 169152-24-3 169152-25-4
169152-26-5 169152-27-6 169152-28-7 169152-29-8 169152-30-1
169152-31-2 169152-32-3 169152-33-4 169152-34-5 169152-35-6
169152-36-7 169152-44-7 169152-45-8 169152-46-9
169152-47-0 169152-48-1 169152-49-2 169152-50-5 169152-51-6
169152-52-7 169152-53-8 169527-92-8

RL: TEM (Technical or engineered material use); USES (Uses)

(display device liq. crystal compns. contg.)

IT 147622-84-2P 147622-85-3P 162785-95-7P 162785-97-9P 162785-98-0P
163671-44-1P 163671-71-4P 163671-94-1P 163672-08-0P 163672-09-1P
163672-10-4P 163672-11-5P 163672-13-7P 163672-14-8P 163672-15-9P
163672-16-0P 163672-17-1P 163672-18-2P 163672-19-3P 163672-20-6P
163672-21-7P 163672-22-8P 163672-23-9P 163672-26-2P 163672-27-3P
169273-18-1P

RL: RCT (Reactant); SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(prepn. and reaction in prepg. liq. crystal for display devices)

IT 162785-83-3P 162785-86-6P 162785-89-9P 162785-90-2P 162785-91-3P
163671-73-6P 163671-84-9P 163671-85-0P 163671-86-1P 163671-87-2P
163671-88-3P 163671-89-4P 163671-90-7P 163671-91-8P 163671-92-9P
163671-93-0P 163671-94-1P 163671-95-2P 163671-96-3P 163671-97-4P
163671-98-5P 163671-99-6P 163672-00-2P 163672-01-3P 163672-02-4P
163672-03-5P 163672-04-6P 163672-06-8P 163672-07-9P 169151-67-1P
169151-68-2P 169151-69-3P 169151-70-6P 169151-71-7P 169151-72-8P
169151-73-9P 169151-74-0P 169151-75-1P 169273-08-9P 169273-09-0P
169273-10-3P 169273-11-4P 169273-12-5P 169273-13-6P 169273-14-7P

169273-15-8P

RL: SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)

(prepn. and use in liq. crystal compns. for display devices)

IT 115-19-5 4894-75-1 40649-36-3 56309-94-5 61203-83-6 82832-73-3

163671-44-1 163671-71-4 163672-25-1

RL: RCT (Reactant); TEM (Technical or engineered material use); RACT (Reactant or reagent); USES (Uses)

(reaction in prepg. liq. crystal for display devices)

IT 169152-36-7

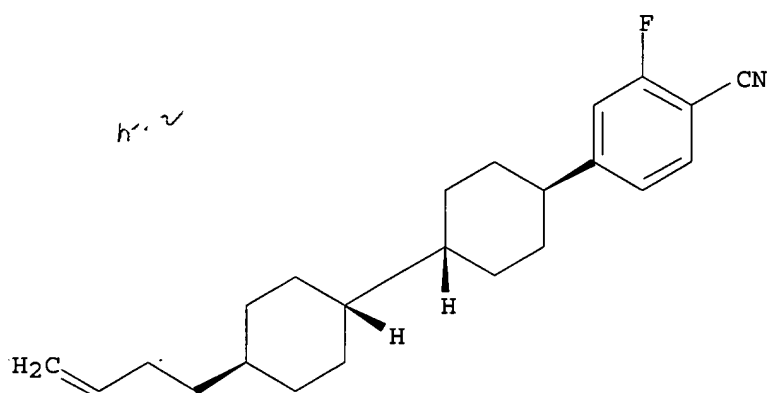
RL: TEM (Technical or engineered material use); USES (Uses)

(display device liq. crystal compns. contg.)

RN 169152-36-7 CAPLUS

CN Benzonitrile, 4-[4'-(3-butenyl)[1,1'-bicyclohexyl]-4-yl]-2-fluoro-,
[trans(trans)]- (9CI) (CA INDEX NAME)

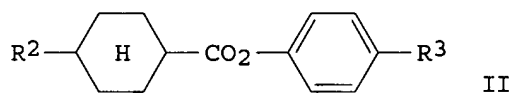
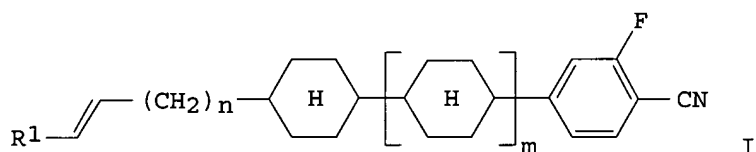
Relative stereochemistry.



AN 1994:567077 CAPLUS
 DN 121:167077
 TI Nematic liquid crystal compositions and liquid-crystal display devices using same
 IN Takeuchi, Kyobumi; Takatsu, Haruyoshi; Maruchin, Shatsuto; Rihyaruto, Buufuetsukaa
 PA Dainippon Ink & Chemicals, Japan; Hoffmann La Roche
 SO Jpn. Kokai Tokkyo Koho, 27 pp.
 CODEN: JKXXAF
 DT Patent
 LA Japanese
 IC ICM C09K019-42
 ICS G02F001-13; G02F001-133
 CC 74-13 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 05311172	A2	19931122	JP 1992-117739	19920511
	JP 3228781	B2	20011112		
PRAI	JP 1992-117739		19920511		

GI



AB The title compns. comprise compds. represented by I and II [R1 = Me, H; n = 0, 2; m = 0, 1; R2 = alkyl, alkenyl; R3 = alkyl, alkoxy, alkenyloxy]. Compds. in addn. to I and II were described in details in the text. The liq.-crystal display devices are of super-twisted nematic LCDs, which use the compns. described above. The compns. exhibited a low threshold value, a fast response time, and high chem. stability.

ST super twisted nematic liq crystal; LCD nematic liq crystal

IT Optical imaging devices

(electrooptical liq.-crystal, super-twisted nematic compns. for)

IT Liquid crystals

(nematic, super-twisted, compns. of)

IT 39969-29-4 73255-62-6 79709-85-6 84016-65-9 84655-98-1
 86503-56-2 87334-49-4 91225-15-9 95973-47-0 98495-10-4
 107949-21-3 107949-31-5 114834-76-3 122705-88-8 155041-85-3
 157453-51-5 157453-52-6 157453-53-7 157453-54-8
 157453-59-3 157453-60-6 157453-61-7 157543-22-1
 157543-23-2 157543-24-3 157543-25-4
 157543-26-5 157543-27-6 157543-28-7
 157543-29-8 157603-92-4

RL: USES (Uses)

(nematic liq. crystal compn. contg.)

IT 157453-52-6 157453-53-7 157543-22-1
 157543-23-2 157543-24-3 157543-25-4
 157543-26-5 157543-27-6 157543-28-7
 157603-92-4

RL: USES (Uses)

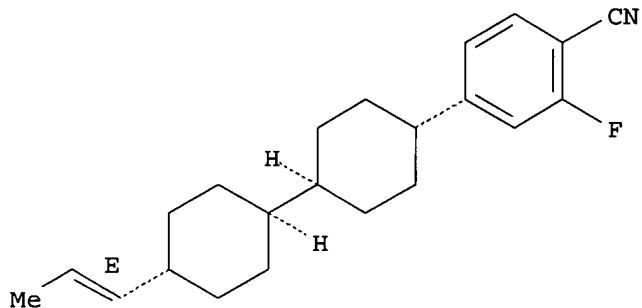
(nematic liq. crystal compn. contg.)

RN 157453-52-6 CAPLUS

CN Benzonitrile, 2-fluoro-4-[4'-(1-propenyl)[1,1'-bicyclohexyl]-4-yl]-, [1'.alpha.(trans),4'.beta.(E)]- (9CI) (CA INDEX NAME)

Relative stereochemistry.

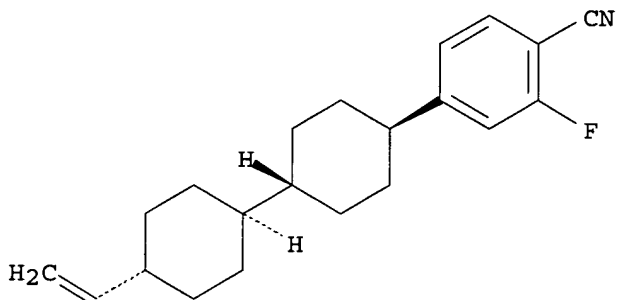
Double bond geometry as shown.



RN 157453-53-7 CAPLUS

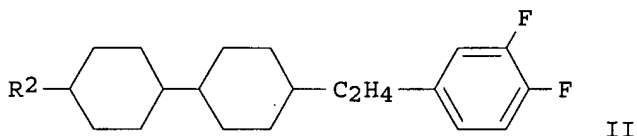
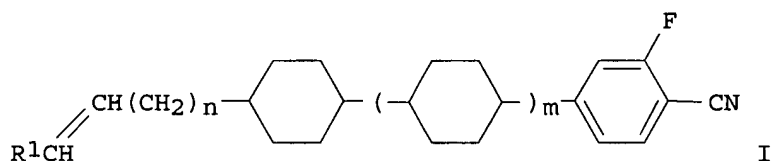
CN Benzonitrile, 4-(4'-ethenyl[1,1'-bicyclohexyl]-4-yl)-2-fluoro-, [trans(trans)]- (9CI) (CA INDEX NAME)

Relative stereochemistry.



AN 1995:543538 CAPLUS
 DN 122:303158
 TI Nematic liquid crystal composition and display using same
 IN Takeuchi, Kyobumi; Takatsu, Haruyoshi; Maruchin, Shatsuto; Rihyaruto, Buufuetsukaa
 PA Dainippon Ink & Chemicals, Japan; Hoffmann La Roche
 SO Jpn. Kokai Tokkyo Koho, 21 pp.
 CODEN: JKXXAF
 DT Patent
 LA Japanese
 IC ICM C09K019-30
 ICS C09K019-34; C09K019-42
 ICA G02F001-13
 CC 74-13 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 06340877	A2	19941213	JP 1992-135141	19920527
	JP 3233684	B2	20011126		
PRAI	JP 1992-135141		19920527		
OS	MARPAT 122:303158				
GI					



AB The title nematic liq. crystal compn. contains I [R1 = H, Me; n = 0, 2; m = 0, 1] and compds. related to II [R2 = C2-7 straight-chain alkyl, alkenyl, CjH2j+1OckH2k (j = 1-3; k = 2-50)]. The compn. is used in super-twisted nematic liq. crystal displays.
 ST nematic liq crystal compn display
 IT Liquid crystals
 (nematic compn.)
 IT Optical imaging devices
 (liq.-crystal, super-twisted nematic)
 IT 163059-54-9 163059-55-0 163059-56-1
 RL: PRP (Properties); TEM (Technical or engineered material use); USES (Uses)
 (nematic liq. crystal compn.)
 IT 82832-57-3 82832-58-4 94819-16-6 94840-77-4 107215-66-7
 109970-65-2 109970-66-3 114834-76-3 117943-37-0 118164-50-4
 119990-81-7 121118-73-8 133937-72-1 134442-19-6 142400-92-8
 143874-14-0 145550-87-4 147671-58-7 148843-06-5 151559-27-2
 151854-71-6 155266-68-5 157453-50-4 157453-51-5 157453-52-6
 157453-53-7 157453-54-8 157453-55-9
 RL: PRP (Properties); TEM (Technical or engineered material use); USES (Uses)
 (nematic liq. crystal compn. contg.)
 IT 163059-55-0 163059-56-1

RL: PRP (Properties); TEM (Technical or engineered material use); USES (Uses)

(nematic liq. crystal compn.)

RN 163059-55-0 CAPLUS

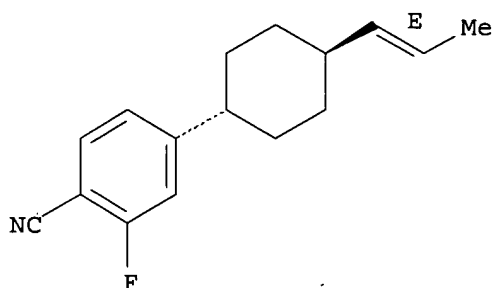
CN Benzonitrile, 4-(4'-ethenyl[1,1'-bicyclohexyl]-4-yl)-2-fluoro-, [trans(trans)]-, mixt. with [trans(trans)]-4-[4'-(3-butenyl)[1,1'-bicyclohexyl]-4-yl]-1,2-difluorobenzene, [trans(trans)]-4-(4'-ethenyl[1,1'-bicyclohexyl]-4-yl)-1,2-difluorobenzene, [1.alpha.,4.beta.(E)]-2-fluoro-4-[4-(3-pentenyl)cyclohexyl]benzonitrile, [1'.alpha.(trans),4'.beta.(E)]-2-fluoro-4-[4'-(1-propenyl)[1,1'-bicyclohexyl]-4-yl]benzonitrile and [1.alpha.,4.beta.(E)]-2-fluoro-4-[4-(1-propenyl)cyclohexyl]benzonitrile (9CI) (CA INDEX NAME)

CM 1

CRN 157453-54-8

CMF C16 H18 F N

Relative stereochemistry.
Double bond geometry as shown.

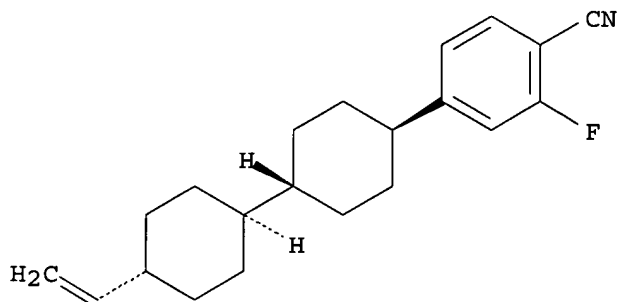


CM 2

CRN 157453-53-7

CMF C21 H26 F N

Relative stereochemistry.

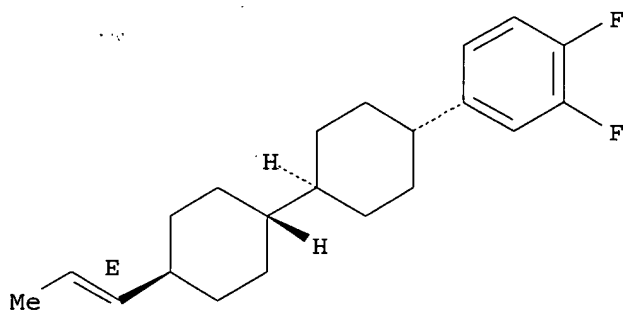


RN 129738-54-1 REGISTRY
 CN Benzene, 1,2-difluoro-4-[(trans,trans)-4'-(1E)-1-propenyl[1,1'-bicyclohexyl]-4-yl]- (9CI) (CA INDEX NAME)
 OTHER CA INDEX NAMES:
 CN Benzene, 1,2-difluoro-4-[4'-(1-propenyl)[1,1'-bicyclohexyl]-4-yl]-, [1'.alpha.(trans),4'.beta.(E)]-
 FS STEREOSEARCH
 MF C21 H28 F2
 CI COM
 SR CA
 LC STN Files: CA, CAPLUS, CHEMLIST, USPATFULL

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C6	C6	6	C6	46.150.1	2
C6	C6	6	C6	46.150.18	1

Relative stereochemistry.
 Double bond geometry as shown.



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	1289224	pH 1	(1) ACD
Bioconc. Factor (BCF)	1289224	pH 4	(1) ACD
Bioconc. Factor (BCF)	1289224	pH 7	(1) ACD
Bioconc. Factor (BCF)	1289224	pH 8	(1) ACD
Bioconc. Factor (BCF)	1289224	pH 10	(1) ACD
Boiling Point (BP)	384.5+/-22.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVP)	60.84+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	157.3+/-18.4 deg C		(1) ACD
Freely Rotatable Bonds (FRB)	3		(1) ACD
H acceptors (HAC)	0		(1) ACD
H donors (HD)	0		(1) ACD
Koc (KOC)	822886	pH 1	(1) ACD
Koc (KOC)	822886	pH 4	(1) ACD
Koc (KOC)	822886	pH 7	(1) ACD
Koc (KOC)	822886	pH 8	(1) ACD
Koc (KOC)	822886	pH 10	(1) ACD

logD (LOGD)	8.34	pH 1	(1) ACD
logD (LOGD)	8.34	pH 4	(1) ACD
logD (LOGD)	8.34	pH 7	(1) ACD
logD (LOGD)	8.34	pH 8	(1) ACD
logD (LOGD)	8.34	pH 10	(1) ACD
logP (LOGP)	8.343+/-0.408		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	318.44		(1) ACD
Vapor Pressure (VP)	9.02E-06 Torr	25.0 deg C	(1) ACD

(1) Calculated using Advanced Chemistry Development (ACD) Software Solaris V4.76 ((C) 1994-2003 ACD)

13 REFERENCES IN FILE CA (1962 TO DATE)
 1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
 13 REFERENCES IN FILE CAPLUS (1962 TO DATE)

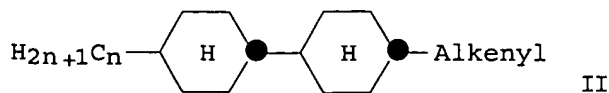
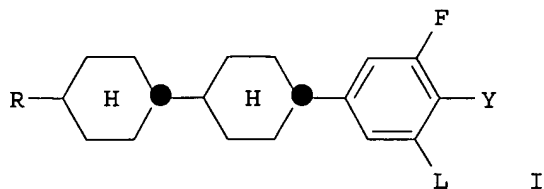
REFERENCE 1

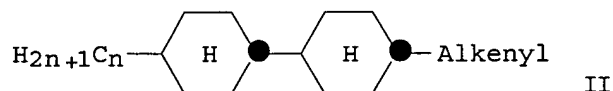
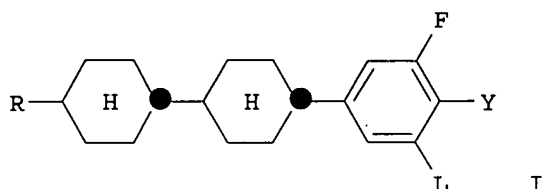
AN 129:252776 CA
 TI Liquid-crystal medium and electrooptical display devices using it
 IN Tarumi, Kazuaki; Schuler, Brigitte; Schwart, Michael; Mackert, Peter J.
 PA Merck Patent G.m.b.H., Germany
 SO Ger. Offen., 18 pp.
 CODEN: GWXXBX
 DT Patent
 LA German
 IC ICM C09K019-08
 ICS C07C043-225; C07C043-192; C07C255-50; C07C255-55; C07C331-28;
 C07C069-76; G02F001-13; G09F009-35
 ICA C09K019-30; C09K019-12; C09K019-14
 CC 75-11 (Crystallography and Liquid Crystals)
 Section cross-reference(s): 25, 74

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 19709890	A1	19980917	DE 1997-19709890	19970311
	GB 2323091	A1	19980916	GB 1998-4981	19980309
	GB 2323091	B2	20011114		
	US 5993692	A	19991130	US 1998-37714	19980310
	JP 10259377	A2	19980929	JP 1998-76430	19980311
PRAI	DE 1997-19709890		19970311		

GI





AB A liq.-crystal medium based on a mixt. of polar compds. having pos. dielec. anisotropy contains .gtoreq.1 compd. of formula I and .gtoreq.1 compd. of formula II, where R = unsubstituted C2-12 alkenyl in which .gtoreq.1 CH2 group may be replaced by O, S, or cyclobutan-1,3-diyl; y = F, Cl, or halogenated C1-6 alkyl, alkenyl, or alkoxy; L = H or F; and n = 1-8.

ST liq crystal medium; electrooptical display liq crystal medium; polar compd liq crystal medium

IT Liquid crystal displays
Liquid crystals
(liq.-crystal medium for electrooptical display devices)

IT 76802-59-0D, PCH 7F, mixt. contg. 129738-34-7D, mixt. contg. 129738-54-1D, mixt. contg. 131819-23-3D, mixt. contg. 133914-49-5D, mixt. contg. 133937-72-1D, mixt. contg. 135734-59-7D, mixt. contg. 135734-60-0D, mixt. contg. 137644-54-3D, mixt. contg. 139215-80-8D, mixt. contg. 139215-88-6D, mixt. contg. 142400-92-8D, mixt. contg. 153429-48-2D, mixt. contg. 173837-35-9D, mixt. contg. 173837-36-0D, mixt. contg. 174805-87-9D, mixt. contg.

RL: DEV (Device component use); TEM (Technical or engineered material use); USES (Uses)
(liq.-crystal medium for electrooptical display devices contg.)

REFERENCE 2

AN 126:39893 CA

TI Liquid crystal composition for electrooptical display device

IN Terashima, Kanetsugu; Takeshita, Fusayuki; Yamamoto, Hitoshi; Kawasyukuda, Hiroaki

PA Chisso Corp., Japan; Terashima, Kanetsugu; Takeshita, Fusayuki; Yamamoto, Hitoshi; Kawasyukuda, Hiroaki

SO PCT Int. Appl., 40 pp.
CODEN: PIXXD2

DT Patent

LA Japanese

IC ICM C09K019-42
ICS C09K019-46

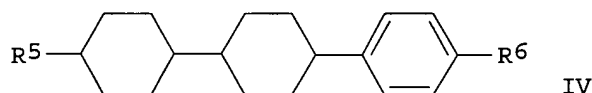
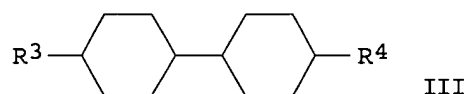
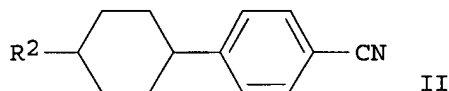
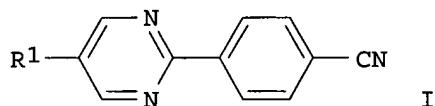
CC 74-13 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)
Section cross-reference(s): 75

FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9634071	A1	19961031	WO 1996-JP193	19960201
W: CN, JP, KR, US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
EP 770663	A1	19970502	EP 1996-901504	19960201
R: CH, DE, GB, LI				
CN 1152331	A	19970618	CN 1996-190392	19960201

TW 424108	B	20010301	TW 1996-85103877	19960402
US 5779933	A	19980714	US 1996-663226	19960617
PRAI JP 1995-101232		19950425		
WO 1996-JP193		19960201		

GI



AB A liq. crystal compn. for electrooptical display device manuf. comprises 1-15% of compds. of formula I, 8-40% of compds. of formula II, 10-30% of compds. of formula III, and 10-45% of compds. of IV wherein R1 represents C1-10 alkyl; R2 represents C1-10 alkyl or C2-10 alkenyl; R3, R6 represent C1-10 alkyl or alkoxy; R4 represents C2-10 alkenyl or alkenyloxy; R5 represents C2-10 alkenyl.

ST liq crystal compn electrooptical display; cyanofluorophenyloxycarbonylbenzene deriv liq crystal display; cyanophenylcyclohexane deriv liq crystal display; cyclohexylcyclohexane deriv liq crystal display

IT Liquid crystal displays
(cyanofluorophenyloxycarbonylbenzene derivs. and related compds. for)

IT	35684-12-9	39969-28-3	39969-29-4	52709-83-8	58743-75-2
	59855-03-7	59855-05-9	61203-99-4	70784-09-7	79709-84-5
	80944-44-1	81782-74-3	85583-83-1	86776-50-3	86776-51-4
	86776-52-5	88038-92-0	95478-15-2	95478-16-3	95480-29-8
	95906-34-6	96184-40-6	96184-42-8	97398-75-9	101478-47-1
	105351-42-6	107949-21-3	116903-48-1	122705-91-3	129738-34-7
	129738-42-7	129738-54-1	136159-76-7	142400-92-8	155041-85-3
	155417-32-6	184652-89-9	184652-90-2	184652-91-3	184652-92-4
	184652-93-5				

RL: DEV (Device component use); TEM (Technical or engineered material use); USES (Uses)
(electrooptical display devices using liq. crystal compns. contg.)

REFERENCE 3

AN 123:355082 CA

TI Orientational ordering of liquid crystals containing a difluoro-substituted phenyl ring

AU Magnuson, Matthew L.; Fung, B. M.; Schadt, Martin

CS Dep. Chem. Biochem., Univ. Oklahoma, Norman, OK, 730919-0370, USA

SO Liquid Crystals (1995), 19(3), 333-8

CODEN: LICRE6; ISSN: 0267-8292

PB Taylor & Francis
DT Journal
LA English
CC 75-11 (Crystallography and Liquid Crystals)
AB The orientational ordering of several liq. crystals contg. a difluoro-substituted Ph ring was studied through the use of C-13 NMR. The fluorinated Ph ring of these liq. crystals have Cs symmetry, so three order parameters are required to completely describe the ordering of this ring. All three of these order parameters were calcd. from C-F dipolar coupling consts. obtained from the C-F splittings in the C-13 NMR spectra. Because of the complexity of the F-coupled spectra, variable angle spinning (VAS) was used to resolve the C-F splittings. To study the orientational ordering over wide ranges of temp., the authors have developed an empirical correlation between the order parameter and the value of a C-F dipolar coupling const. This enabled the authors to study the change in the order parameter with temp. The results of applying this method to several structurally similar liq. crystals contg. the same type of difluorinated Ph ring are presented. A comparison is made to a similar mono-fluorinated liq. crystal.

ST orientational ordering liq crystal fluorophenyl ring
IT Liquid crystals
(difluoro-substituted Ph ring system; orientational ordering of)
IT 82832-57-3 129738-46-1 129738-54-1 170806-75-4
RL: PEP (Physical, engineering or chemical process); PROC (Process)
(orientational ordering of liq. crystals of)

REFERENCE 4

AN 123:326312 CA
TI Polar nematic trans-4-substituted-cyclohexyl (E)-alk-2-enoates. The influence of dipoles and double bonds on the transition temperatures and other physical properties
AU Kelly, S. M.; Schadt, M.; Seiberle, H.
CS Dep. RLCR, F. Hoffmann-La Roche Ltd., Basle, CH-4002, Switz.
SO Liquid Crystals (1995), 18(4), 581-94
CODEN: LICRE6; ISSN: 0267-8292
PB Taylor & Francis
DT Journal
LA English
CC 75-11 (Crystallography and Liquid Crystals)
AB As part of a systematic study of the factors affecting nematic phase formation, the influence of introducing dipoles (as O, carbonyl and carboxy groups) and steric restrictions (as C-C double bonds) in various positions, configuration and combinations in a model system (4-[trans-4-pentylcyclohexyl]benzonitrile) was studied. The authors have introduced an ester group and a C-C double bond with a trans-configuration (E) into the terminal alkyl chain attached to the cyclohexyl ring of a variety of two- and three-ring nematic mesogens of pos. dielec. anisotropy. This is a new combination of a polar ester group (dipole effect) and the added rigidity imposed by the double bond (steric effect). Most of the new (E)-alk-2-enoates contg. two rings in the mol. core possess high m.ps. Only a few two-ring esters exhibit a nematic phase, although the clearing point of those esters exhibiting mesomorphic behavior was high. The corresponding three-ring (E)-alk-2-enoates incorporating an addnl. Ph or cyclohexane ring also possess high melting and clearing points, as well as wide nematic ranges. No smectic mesophases could be obsd. for any of the (E)-alk-2-enoates synthesized. Comparisons with the corresponding derivs. incorporating either just an ester group, or just a C-C double bond in the same position indicate that synergetic effects lead to higher clearing points than would otherwise were expected. The new (E)-alk-2-enoates possess a surprisingly moderate viscosity for esters. The high value of the elastic const. ratio k_{33}/k_{11} is of advantage for mixts. designed for supertwisted nematic LCDs.

ST polar nematic cyclohexyl alkenoate mesomorphism dielec
 IT Viscosity
 (of polar nematic alkylcyclohexyl alkenoates)
 IT Liquid crystals
 (nematic, alkylcyclohexyl alkenoates; influence of dipoles and double
 bonds on transition temps. and other phys. properties of)
 IT 105026-21-9 129738-54-1 133622-74-9 140922-68-5
 RL: PEP (Physical, engineering or chemical process); PROC (Process)
 (liq. crystal properties of mixt. of difluorophenylbicyclohexyl
 butenoate with)
 IT 118164-51-5 127927-93-9 136159-79-0 157396-56-0 157396-57-1
 157396-58-2 157396-59-3 157396-60-6 157396-61-7 157396-62-8
 157396-76-4 157396-77-5 157396-78-6 157396-79-7 164592-00-1
 164592-01-2 164592-02-3 164592-03-4 164592-04-5 164592-05-6
 164592-06-7 164592-07-8 164592-08-9 164592-09-0
 RL: PEP (Physical, engineering or chemical process); PRP (Properties);
 PROC (Process)
 (prepn. and liq. crystal properties and heat of transition of)
 IT 87073-95-8 136159-78-9 157396-75-3 164591-91-7 164591-92-8
 164591-93-9 164591-94-0 164591-95-1 164591-96-2 164591-97-3
 164591-98-4 164591-99-5
 RL: PEP (Physical, engineering or chemical process); PRP (Properties);
 PROC (Process)
 (prepn. and m.p. and heat of transition of)

REFERENCE 5

AN 123:325995 CA
 TI The effect of molecular association and tube dilation on the rotational
 viscosity and rotational diffusion in nematic liquid crystals
 AU Raviol, A.; Stille, W.; Strobl, G.
 CS Fak. Phys., Univ. Freiburg, Freiburg, D-79104, Germany
 SO Journal of Chemical Physics (1995), 103(9), 3788-94
 CODEN: JCPSA6; ISSN: 0021-9606
 PB American Institute of Physics
 DT Journal
 LA English
 CC 75-1 (Crystallography and Liquid Crystals)
 Section cross-reference(s): 65
 AB A combination of director reorientation expts. with dielec. relaxation
 spectroscopy was used to study the relation between the rotational
 viscosity γ_1 and the rotational diffusion consts. in nematic compds.
 with different assocn. tendency. Increased values for γ_1 were found
 for compds. showing strong assocn. This is explained by increased
 rotational friction of the assocn. due to the necessary translational
 motion of the mols. within these groups. For nonassocg. compds., γ_1
 is described quant. by Marrucci's theory, when the tube dilation effect
 described by Doi for the rotational diffusion in an orientationally
 ordered environment is taken into account.
 ST rotational viscosity diffusion nematic liq crystal
 IT Liquid crystals
 (nematic, effect of mol. assocn. and tube dilation on rotational
 viscosity and rotational diffusion in)
 IT Diffusion
 Viscosity
 (rotational, effect of mol. assocn. and tube dilation on rotational
 viscosity and rotational diffusion in)
 IT 40817-08-1, 5CB 61204-01-1, PCH5 129738-54-1 140922-68-5
 170656-12-9
 RL: PEP (Physical, engineering or chemical process); PROC (Process)
 (effect of mol. assocn. and tube dilation on rotational viscosity and
 rotational diffusion in nematic liq. crystals of)

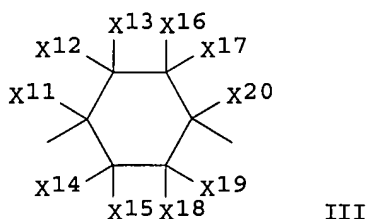
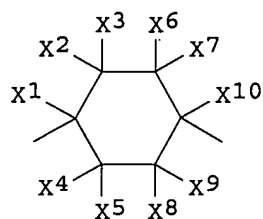
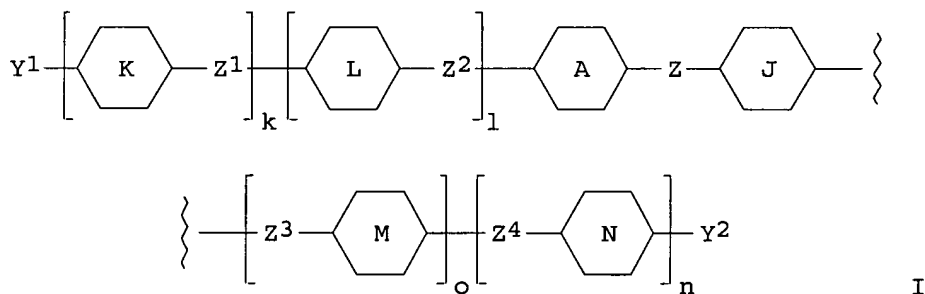
REFERENCE 6

AN 123:301635 CA
 TI Cyclic hydrocarbon derivative and liquid crystal composition containing the same.
 IN Takatsu, Haruyoshi; Takehara, Sadao; Takeuchi, Kiyohumi; Osawa, Masashi; Ogawa, Shinji; Ishida, Norie
 PA Dainippon Ink Chemical Industry Co., Japan
 SO Eur. Pat. Appl., 334 pp.
 CODEN: EPXXDW
 DT Patent
 LA English
 IC ICM C09K019-04
 ICS C09K019-30; C07B059-00; C07C255-50; C07C043-20; C07C025-18
 CC 74-13 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)
 Section cross-reference(s): 75

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 637623	A1	19950208	EP 1994-111448	19940722
	EP 637623	B1	20011004		
	R: DE, GB				
	JP 07034066	A2	19950203	JP 1993-182734	19930723
	US 5474707	A	19951212	US 1994-278260	19940721
	US 5536443	A	19960716	US 1995-429485	19950425
PRAI	JP 1993-182734		19930723		
	US 1994-278260		19940721		

GI



AB A novel cyclic hydrocarbon deriv. is disclosed, which is represented by formula I, wherein Y1 and Y2 each independently represent F, Cl, CN, OCN, SCN, OCF3, OCF2H, OCH2CF3, CF3, R, OR, CO2R, or -OCOR, wherein R represents alkyl having 1-20 C atoms, alkenyl having from 2-20 C atoms, or alkoxyalkyl having 2-20 C atoms, provided that at least one of Y1 and Y2 represents R, OR, CO2R, or -OCOR; Z, Z1-4 each independently represent a single bond, CH2CH2, CH=CH, C.tplbond.C, CO2, OCO, CH2O, OCH2, (CH2)4, (CH2)3O, or O(CH2)3; ring A represents a group of formula II, wherein X1-10 each independently represent H or D, provided that at least one of

them represents D; rings K, L, J, M, N each independently represent trans-1,4-cyclohexylene, 1,4-cyclohexenylene, trans-1,4-phenylene, 1,4-phenylene substituted with 1-4 substituents selected from F, Cl, CN, and CH₃, 1,3-dioxane-2,6-diyl, pyrimidine-2,5-diyl, pyridine-2,5-diyl, or a group of formula III, wherein X₁₁₋₂₀ each independently represent H or D, provided that at least one of them represents D; k, l, m, n each independently represent 0 or 1 with the sum of k, l, m, and n being 0, 1, or 2 is prep'd. and used in a liq. crystal compn. for an electrooptical display device.

ST cyclic hydrocarbon liq crystal display

IT Liquid crystals

(cyclic hydrocarbons as)

IT Optical imaging devices

(electrooptical, liq. crystal compns. contg. cyclic hydrocarbons for)

IT 169273-07-8 169273-17-0 169273-19-2 169273-20-5 169273-21-6
169527-81-5 169527-83-7 169527-84-8 169527-85-9 169527-86-0
169527-87-1 169527-88-2 169527-89-3 169527-90-6 169527-91-7
169532-92-7

RL: TEM (Technical or engineered material use); USES (Uses)

(display device liq. crystal compn.)

IT 61203-99-4 61204-01-1 61204-03-3 67589-39-3 67589-41-7
67589-46-2 67589-47-3 67589-52-0 67589-53-1 86504-59-8
92118-81-5 92118-82-6 92118-83-7 92118-84-8 93743-04-5
94819-16-6 94840-77-4 96042-33-0 97941-21-4 119990-81-7
129738-54-1 142400-92-8 144916-76-7 147065-76-7 155041-85-3
155266-68-5 159586-97-7 162785-84-4 162785-85-5 163671-84-9
163671-92-9 163671-97-4 167949-21-5 167949-22-6 167949-24-8
167949-26-0 167949-27-1 169151-78-4 169151-79-5 169151-80-8
169151-81-9 169151-82-0 169151-83-1 169151-84-2 169151-85-3
169151-86-4 169151-87-5 169151-88-6 169151-89-7 169151-90-0
169151-91-1 169151-92-2 169151-93-3 169151-94-4 169151-95-5
169151-96-6 169151-97-7 169151-98-8 169151-99-9 169152-00-5
169152-01-6 169152-02-7 169152-03-8 169152-04-9 169152-05-0
169152-06-1 169152-07-2 169152-08-3 169152-09-4 169152-10-7
169152-11-8 169152-12-9 169152-13-0 169152-14-1 169152-15-2
169152-16-3 169152-17-4 169152-18-5 169152-19-6 169152-20-9
169152-21-0 169152-22-1 169152-23-2 169152-24-3 169152-25-4
169152-26-5 169152-27-6 169152-28-7 169152-29-8 169152-30-1
169152-31-2 169152-32-3 169152-33-4 169152-34-5 169152-35-6
169152-36-7 169152-44-7 169152-45-8 169152-46-9 169152-47-0
169152-48-1 169152-49-2 169152-50-5 169152-51-6 169152-52-7
169152-53-8 169527-92-8

RL: TEM (Technical or engineered material use); USES (Uses)

(display device liq. crystal compns. contg.)

IT 147622-84-2P 147622-85-3P 162785-95-7P 162785-97-9P 162785-98-0P
163671-44-1P 163671-71-4P 163671-94-1P 163672-08-0P 163672-09-1P
163672-10-4P 163672-11-5P 163672-13-7P 163672-14-8P 163672-15-9P
163672-16-0P 163672-17-1P 163672-18-2P 163672-19-3P 163672-20-6P
163672-21-7P 163672-22-8P 163672-23-9P 163672-26-2P 163672-27-3P
169273-18-1P

RL: RCT (Reactant); SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(prepn. and reaction in prepg. liq. crystal for display devices)

IT 162785-83-3P 162785-86-6P 162785-89-9P 162785-90-2P 162785-91-3P
163671-73-6P 163671-84-9P 163671-85-0P 163671-86-1P 163671-87-2P
163671-88-3P 163671-89-4P 163671-90-7P 163671-91-8P 163671-92-9P
163671-93-0P 163671-94-1P 163671-95-2P 163671-96-3P 163671-97-4P
163671-98-5P 163671-99-6P 163672-00-2P 163672-01-3P 163672-02-4P
163672-03-5P 163672-04-6P 163672-06-8P 163672-07-9P 169151-67-1P
169151-68-2P 169151-69-3P 169151-70-6P 169151-71-7P 169151-72-8P
169151-73-9P 169151-74-0P 169151-75-1P 169273-08-9P 169273-09-0P
169273-10-3P 169273-11-4P 169273-12-5P 169273-13-6P 169273-14-7P
169273-15-8P

RL: SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)

(prepn. and use in liq. crystal compns. for display devices)

IT 115-19-5 4894-75-1 40649-36-3 56309-94-5 61203-83-6 82832-73-3
163671-44-1 163671-71-4 163672-25-1

RL: RCT (Reactant); TEM (Technical or engineered material use); RACT (Reactant or reagent); USES (Uses)

(reaction in prep. liq. crystal for display devices)

REFERENCE 7

AN 123:156546 CA

TI Liquid crystal-polymer composite material

IN Coates, David; Greenfield, Simon

PA Merck Patent G.m.b.H., UK

SO Brit. UK Pat. Appl., 37 pp.

CODEN: BAXXDU

DT Patent

LA English

IC ICM C09K019-30

ICS C09K019-14; C09K019-52

CC 74-13 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)

Section cross-reference(s): 75

FAN. CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	GB 2281566	A1	19950308	GB 1994-17672	19940902
	GB 2281566	B2	19980513		
	GB 2292745	A1	19960306	GB 1995-4656	19950308
	GB 2292745	B2	19980819		
PRAI	EP 1993-114037		19930902		
	GB 1994-17672		19940902		

AB The invention refers to a composite material comprising a liq. crystal material (with a birefringence $\Delta n = n_e - n_o$) and a polymeric medium (which is optically substantially transparent and isotropic and has a refractive index of nm) wherein either the liq. crystal material is embedded in micro-droplets in the polymeric medium (with one of the refractive indexes of the liq. crystal material being substantially matched to the refractive index nm of said polymeric medium) or the liq. crystal material is present as a substantially continuous phase in a 3-dimensional network formed by or with the polymeric medium, the composite being characterized in that the liq. crystal material contains at least one compd. of formula $R_1-CH:CH-R_2-(A-Z)_m-B-R_3$ [wherein R_1 is alkyl with 1-6 C atoms, wherein one or two CH_2 -groups can be replaced by -O- or -CO-; R_2 is alkylated $(CH_2)_p$ - with p ranging from 1-6, wherein one or two CH_2 -groups can be replaced by -O- or -CO-; A is independently from each other Z is independently from each other a single bond, -CH₂-CH₂-, COO- or -OCO-; m is 1, 2 or 3; B is R₃ is F, Cl, CN, X-G; X is a single bond, -O- or -S-; G is Me or Et where one or more H may be replaced by F; with the proviso that at least one of A and B is a laterally mono- or difluorinated 1,4-phenylene group]. The precursor of the composite materials is also claimed, namely a compn. comprising a liq. crystal material (which contains at least one compd. of formula) and a UV-curable precursor of the polymeric medium.

ST liq crystal polymer composite material

IT Optical instruments

(electrooptical switches, liq. crystal-polymer composite material for)

IT 129738-46-1 129738-54-1 157453-54-8 163004-89-5 166743-95-9
166743-96-0 166743-97-1 166743-98-2 166743-99-3 166744-00-9
166744-01-0 166744-02-1 166744-03-2 166744-04-3 166744-05-4
166744-06-5

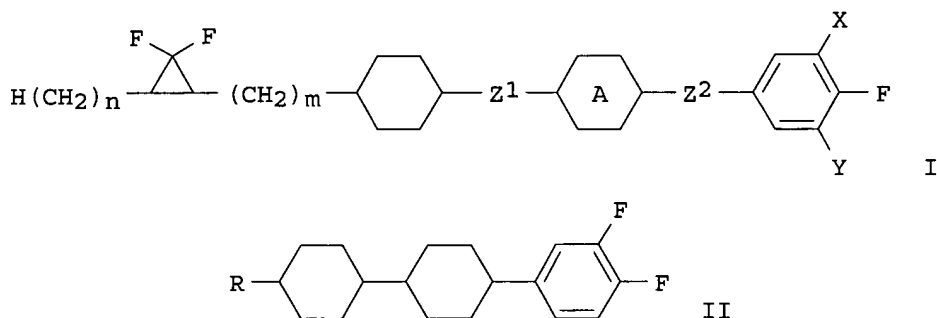
RL: DEV (Device component use); PRP (Properties); USES (Uses)

(contained in liq. crystal-polymer composite material for switch)

REFERENCE 8

AN 122:21002 CA
 TI Preparation of difluorocyclopropane derivatives as liquid crystals
 IN Takehara, Sadao; Ogawa, Shinji; Takatsu, Haruyoshi
 PA Dainippon Ink & Chemicals, Japan
 SO Jpn. Kokai Tokkyo Koho, 15 pp.
 CODEN: JKXXAF
 DT Patent
 LA Japanese
 IC ICM C07C025-18
 ICS C09K019-30
 CC 75-11 (Crystallography and Liquid Crystals)
 Section cross-reference(s): 74
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 06184020	A2	19940705	JP 1993-202370	19930816
PRAI	JP 1992-282873		19921021		
GI					



AB The title compds. (I; m = 0-5; n = 0-7; Z1, Z2 = single bond or CH2CH2, provided that at least one of Z1 and Z2 = single bond; ring A = trans-1,4-cyclohexylene or 1,4-phenylene; X, Y = H, F), useful for liq. crystal switching devices for displays and particularly useful as active matrix-driving liq. crystal materials, are prepd. A liq. crystal compn. contains at least one I. (Difluorocyclopropyl)cyclohexane and [(difluorocyclopropyl)alkyl]cyclohexane derivs. I show good compatibility with widely used nematic mother liq. crystals, small refractive index anisotropy, and excellent chem. stability owing to the absence of polar groups such as cyano and ester groups, and can provide liq. crystal compns. showing nematic liq. crystal phase at wide temp. range, relatively small refractive index anisotropy and threshold voltage, and high specific resistance and voltage holding ratio when they are added to a liq. crystal compn. Thus, 2.0 g (trans-1-propenyl)bicyclohexane deriv. (trans,trans-II; R = trans-1-propenyl) was dissolved in diethylene glycol di-Me ether followed by adding 10 mg 3,5-di-tert-butylcatechol and after heating the soln. to 165.degree., a soln. of sodium chlorodifluoroacetate in the same solvent was added dropwise over 45 min while the temp. was kept at .gtoreq.160.degree. followed by heating the resulting mixt. at 165.degree. for 2 h to give all trans-II (R = 2,2-difluoro-3-methylcyclopropyl). A liq. crystal compn. contg. 30 wt.% II (R = 3-ethyl-2,2-difluorocyclopropylmethyl) and an active-matrix mother liq. crystal (70 wt.%) consisting of 50% 4-[4-(4-vinylcyclohexyl)cyclohexyl]-1,2-difluorobenzene and 50% 4-[4-[4-(3-buten-1-yl)vinylcyclohexyl]cyclohexyl]-1,2-difluorobenzene showed the upper limit

temp. of nematic phase at 96.9.degree., dielec. const. anisotropy (.DELTA..epsilon.) 4.6, refractive index anisotropy (.DELTA.n) 0.082, and threshold voltage (Vth) 2.16 V in a twisted nematic cell vs. 116.7.degree., .DELTA..epsilon. = 4.7, .DELTA.n = 0.082, and Vth = 2.43 V, resp., for the mother liq. crystal.

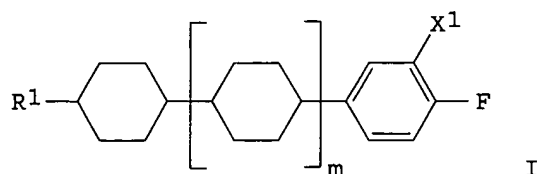
- ST fluorocyclopropane deriv prepn liq crystal; fluorocyclopropylcyclohexane prepn liq crystal; fluorocyclopropylalkylcyclohexane prepn liq crystal
- IT Liquid crystals
(prepn. of (difluorocyclopropyl)cyclohexane and [(difluorocyclopropyl)alkyl]cyclohexane derivs. as liq. crystals)
- IT Optical imaging devices
(electrooptical liq.-crystal, prepn. of (difluorocyclopropyl)cyclohexane and [(difluorocyclopropyl)alkyl]cyclohexane derivs. as liq. crystals for (active matrix) nematic liq. crystal displays)
- IT 1895-39-2, Sodium chlorodifluoroacetate
RL: RCT (Reactant); RACT (Reactant or reagent)
(difluorocarbene insertion with alkenylcyclohexane derivs. in prepn. of (difluorocyclopropyl)cyclohexane or [(difluorocyclopropyl)alkyl]cyclohexane derivs. as liq. crystal)
- IT 129738-54-1 159586-94-4 159586-95-5 159586-96-6 159586-97-7
159652-71-8 159652-72-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(difluorocarbene insertion with sodium chlorodifluoroacetate in prepn. of (difluorocyclopropyl)cyclohexane or [(difluorocyclopropyl)alkyl]cyclohexane deriv. as liq. crystal)
- IT 159652-67-2 159652-68-3 159652-69-4 159652-70-7 159700-01-3
RL: DEV (Device component use); USES (Uses)
(nematic liq. crystal compn. for active-matrix liq. crystal displays)
- IT 61203-99-4 61204-01-1 61204-03-3 67589-39-3 67589-41-7
67589-46-2 67589-47-3 67589-52-0 67589-53-1 159652-66-1
RL: DEV (Device component use); USES (Uses)
(nematic liq. crystal compn. for liq. crystal displays)
- IT 159586-89-7P 159586-90-0P 159586-91-1P 159586-92-2P 159586-93-3P
159652-64-9P 159652-65-0P
RL: DEV (Device component use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(prepn. of (difluorocyclopropyl)cyclohexane or [(difluorocyclopropyl)alkyl]cyclohexane derivs. as liq. crystals for (active matrix) nematic liq. crystal displays)

REFERENCE 9

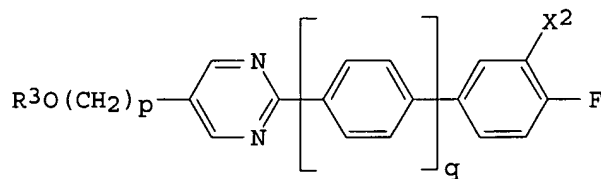
AN 120:311802 CA
TI Nematic liquid crystal composition
IN Takeuchi, Kyobumi; Takatsu, Haruyoshi; Takehara, Sadao; Oosawa, Masashi
PA Dainippon Ink & Chemicals, Japan
SO Jpn. Kokai Tokkyo Koho, 10 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
IC ICM C09K019-42
ICS G02F001-13
CC 74-13 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 05148483	A2	19930615	JP 1991-312448	19911127
PRAI	JP 1991-312448		19911127		
GI					



I



II

AB A nematic liq. crystal compn. comprises a compd. I [R1 = C2-5 linear alkyl, C2-5 linear alkenyl, R2-O(CH2)k-; R2 = C1-3 linear alkyl; k = 1-6; m = 0, 1; X1 = H, F] and a compd. II [R3 = C1-3 linear alkyl; p = 1-6; q = 0, 1; X2 = H, F]. Preferably, the refractive index of the compn. falls in the range of 0.07-0.11. An active matrix LCD using this compn. is free of flickers, and provides a high pretilt angle.

ST nematic liq crystal compn; active matrix LCD display

IT Optical imaging devices
(electrooptical liq.-crystal, active matrix, nematic compn. for)

IT Liquid crystals
(nematic, compn. of)

IT 82832-27-7 119990-81-7 122705-88-8 129738-54-1 133622-71-6
133622-72-7 133622-74-9 137189-60-7 137326-40-0 142400-92-8
146862-12-6 155041-85-3

RL: USES (Uses)
(nematic liq. crystal compn. contg.)

REFERENCE 10

AN 120:120874 CA

TI Liquid crystal composition containing diphenylacetylene and 1-cyclohexyl-4-phenylcyclohexane derivatives and display devices using them

IN Kotani, Kunihiro; Ootsuka, Tetsuo; Fujita, Yutaka; Oonishi, Hiroyuki; Shirokura, Sayuri

PA Rodeitsuku Kk, Japan

SO Jpn. Kokai Tokkyo Koho, 14 pp.
CODEN: JKXXAF

DT Patent

LA Japanese

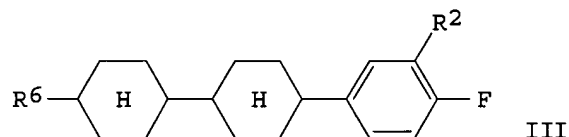
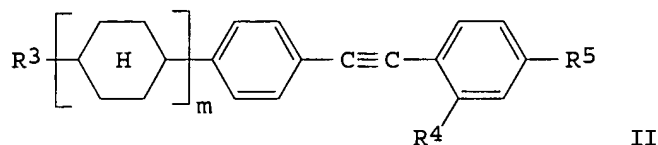
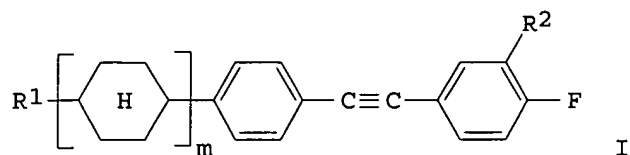
IC ICM C09K019-30
ICS C09K019-42; G02F001-13

CC 74-13 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)
Section cross-reference(s): 75

FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 05059364	A2	19930309	JP 1991-220695	19910830
JP 3128880	B2	20010129		
PRAI JP 1991-220695		19910830		

GI



AB A liq. crystal compn. contains .gtoreq.1 compd. selected from .gtoreq.2 groups of compds. including diphenylacetylene derivs. I and II (R1, R3 = C1-10 alkyl; R2 = H, F; R4 = H, F, Me; R5 = C1-10 alkyl or alkoxy; m = 0, 1) and 1-cyclohexyl-4-phenylcyclohexane derivs. III (R6 = C1-10 alkyl, alkenyl, ether; R2 = H, F) which is used in a liq. crystal device. The liq. crystal compn. shows low viscosity, high speed response, and high refractive index anisotropy (.DELTA.n) without decrease in chem. stability and voltage retention rate and is suitable for active-matrix display.

ST liq crystal compn diphenylacetylene cyclohexylphenylcyclohexane; active matrix display liq crystal

IT Liquid crystals

(compns., contg. diphenylacetylene and cyclohexylphenylcyclohexane derivs.)

IT Optical imaging devices

(electrooptical liq.-crystal, active-matrix, compns. contg. diphenylacetylene and cyclohexylphenylcyclohexane derivs. for)

IT 39969-28-3 39969-29-4 85583-83-1 107949-21-3 107949-22-4
107949-29-1 107949-31-5 109970-65-2 109970-66-3 114834-76-3
114834-78-5 121118-73-8

RL: USES (Uses)

(liq. crystal compn. contg., for active-matrix display devices)

IT 82832-27-7 86504-59-8 119990-81-7 119990-82-8 129738-54-1
133622-72-7 133622-74-9 142400-92-8 152208-71-4 152208-72-5
152695-38-0 153061-64-4

RL: TEM (Technical or engineered material use); USES (Uses)

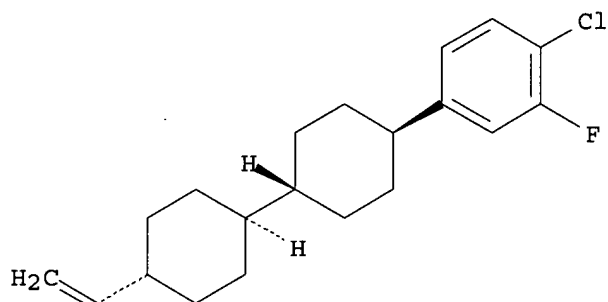
(liq. crystal compn., for active-matrix display devices)

RN 139778-51-1 REGISTRY
 CN Benzene, 1-chloro-4-(4'-ethenyl[1,1'-bicyclohexyl]-4-yl)-2-fluoro-,
 [trans(trans)]- (9CI) (CA INDEX NAME)
 FS STEREOSEARCH
 MF C20 H26 Cl F
 SR CA
 LC STN Files: CA, CAPLUS, USPATFULL

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
=====	=====	=====	=====	=====	=====
C6	C6	6	C6	46.150.1	2
C6	C6	6	C6	46.150.18	1

Relative stereochemistry.



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
=====	=====	=====	=====
Bioconc. Factor (BCF)	1335769	pH 1	(1) ACD
Bioconc. Factor (BCF)	1335769	pH 4	(1) ACD
Bioconc. Factor (BCF)	1335769	pH 7	(1) ACD
Bioconc. Factor (BCF)	1335769	pH 8	(1) ACD
Bioconc. Factor (BCF)	1335769	pH 10	(1) ACD
Boiling Point (BP)	392.8+/-22.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	61.75+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	226.9+/-15.1 deg C		(1) ACD
Freely Rotatable Bonds (FRB)	3		(1) ACD
H acceptors (HAC)	0		(1) ACD
H donors (HD)	0		(1) ACD
Koc (KOC)	844045	pH 1	(1) ACD
Koc (KOC)	844045	pH 4	(1) ACD
Koc (KOC)	844045	pH 7	(1) ACD
Koc (KOC)	844045	pH 8	(1) ACD
Koc (KOC)	844045	pH 10	(1) ACD
logD (LOGD)	8.36	pH 1	(1) ACD
logD (LOGD)	8.36	pH 4	(1) ACD
logD (LOGD)	8.36	pH 7	(1) ACD
logD (LOGD)	8.36	pH 8	(1) ACD
logD (LOGD)	8.36	pH 10	(1) ACD
logP (LOGP)	8.363+/-0.326		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD

Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	320.87		(1) ACD
Vapor Pressure (VP)	5.05E-06 Torr	25.0 deg C	(1) ACD

(1) Calculated using Advanced Chemistry Development (ACD) Software Solaris V4.76 ((C) 1994-2003 ACD)

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

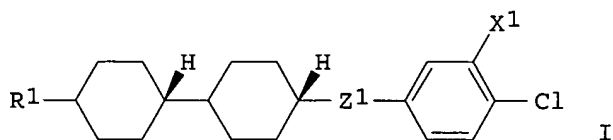
REFERENCE 1

AN 116:151296 CA
TI Preparation of [[(chlorophenyl)cyclohexyl]cyclohexyl]alkenes as liquid crystals
IN Buchecker, Richard; Germann, Alfred; Schadt, Martin; Villiger, Alois
PA Hoffmann-La Roche, F., A.-G., Switz.
SO Eur. Pat. Appl., 17 pp.
CODEN: EPXXDW
DT Patent
LA German
IC ICM C07C025-24
ICS C09K019-30
CC 25-3 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 75

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 458176	A1	19911127	EP 1991-107829	19910515
	EP 458176	B1	19950802		
	R: CH, DE, FR, GB, IT, LI, NL				
	JP 04226929	A2	19920817	JP 1991-140668	19910517
	US 5174921	A	19921229	US 1991-701728	19910520
PRAI	CH 1990-1718		19900521		

GI



AB Title compds. (I; Z1 = bond, CH₂CH₂; X1 = H, F, Cl; R1 = 1E-alkenyl), were prepd. Thus, Grignard reaction of 4-bromo-1-chlorobenzene with 8-(4-oxocyclohexyl)-1,4-dioxaspiro[4.5]decane gave 1-(4-chlorophenyl)-4-(1,4-dioxa-8-spiro[4.5]docyl)cyclohexanol, which was converted to trans-4'-(4-chlorophenyl)[1,1'-bicyclohexyl]-4-one in several steps. Wittig reaction of the latter with MeOCH₂PPh₃Cl followed by hydrolysis gave trans-4'-(4-chlorophenyl)-[1,1'-bicyclohexyl]-trans-4-carboxaldehyde. Wittig reaction of the latter with EtPPh₃Br gave an 11:88 E/Z mixt. of propanes, which was heated with 2N HCl and Na benzenesulfinate in PhMe to give 1-[trans-4-[trans-4-(1E-propenyl)cyclohexyl]cyclohexyl]-4-chlorobenzene (II). A mixt. contg. 90 wt.% 4-(trans-4-pentylcyclohexyl)benzonitrile and 10 wt.% II in a low bias tilt cell showed V₁₀ = 1.66 V, ton = 27 ms, toff = 36 ms, and Δn = 0.127.

ST chlorophenyldicyclohexane prepn liq crystal; electrooptical display component chlorophenyldicyclohexane

IT Liquid crystals

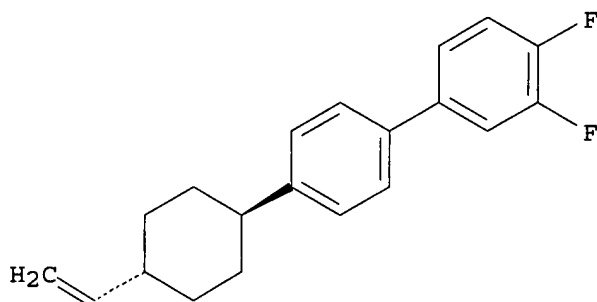
([[(chlorophenyl)cyclohexyl]cyclohexyl]alkenes)
 IT Optical imaging devices
 (electro-, liq.-crystal, [[(chlorophenyl)cyclohexyl]cyclohexyl]alkene
 for)
 IT 4894-75-1, 4-Phenylcyclohexanone
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (Friedel-Crafts reaction of, with oxalyl chloride)
 IT 79-37-8, Oxalyl chloride
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (Friedel-Crafts reaction of, with phenylcyclohexanone)
 IT 106-39-8, 4-Bromo-1-chlorobenzene
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (Grignard reaction of, with (oxocyclohexyl)dioxaspirodecane, in prepn.
 of liq. crystal)
 IT 56309-94-5
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (Grignard reaction of, with bromochlorobenzene, in prepn. of liq.
 crystal)
 IT 4009-98-7, Methoxymethyltriphenylphosphonium chloride
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (Wittig reaction of, with chlorophenylcyclohexylcyclohexanone, in
 prepn. of liq. crystal)
 IT 622-95-7, 4-Chlorobenzyl bromide
 RL: PROC (Process)
 (conversion of, to triphenylphosphonium salt)
 IT 51044-12-3P, 4-Chlorobenzyltriphenylphosphonium bromide
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (prepn. and Wittig reaction of, with dioxolanylcyclohexylcyclohexylcarb
 oxaldehyde, in prepn. of liq. crystal)
 IT 139778-75-9P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (prepn. and esterification of, in prepn. of
 chlorophenylcyclohexylcyclohexane liq. crystal)
 IT 137464-98-3P 139778-59-9P 139778-60-2P 139778-61-3P 139778-62-4P
 139778-63-5P 139778-64-6P 139778-65-7P 139778-66-8P 139778-67-9P
 139778-68-0P 139778-69-1P 139778-70-4P 139778-71-5P 139778-72-6P
 139778-73-7P 139778-74-8P 139894-93-2P 139894-94-3P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of, as intermediate for chlorophenylbicyclohexane liq. crystal)
 IT 139778-48-6P 139778-49-7P 139778-50-0P 139778-51-1P 139778-52-2P
 139778-53-3P 139778-54-4P 139778-55-5P 139778-56-6P 139778-57-7P
 139778-58-8P 139879-90-6P 139879-91-7P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of, as liq. crystal)
 IT 1530-32-1, Ethyltriphenylphosphonium bromide
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with chlorophenylcyclohexylcyclohexylcarboxaldehyde, in
 prepn. of liq. crystal)

RN 142256-81-3 REGISTRY
 CN 1,1'-Biphenyl, 4'-(4-ethenylcyclohexyl)-3,4-difluoro-, trans- (9CI) (CA
 INDEX NAME)
 FS STEREOSEARCH
 MF C20 H20 F2
 CI COM
 SR CA
 LC STN Files: CA, CAPLUS, USPATFULL

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C6	C6	6	C6	46.150.1	1
C6	C6	6	C6	46.150.18	2

Relative stereochemistry.



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	122102	pH 1	(1) ACD
Bioconc. Factor (BCF)	122102	pH 4	(1) ACD
Bioconc. Factor (BCF)	122102	pH 7	(1) ACD
Bioconc. Factor (BCF)	122102	pH 8	(1) ACD
Bioconc. Factor (BCF)	122102	pH 10	(1) ACD
Boiling Point (BP)	386.4+/-22.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	61.05+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	158.3+/-18.4 deg C		(1) ACD
Freely Rotatable Bonds (FRB)	3		(1) ACD
H acceptors (HAC)	0		(1) ACD
H donors (HD)	0		(1) ACD
Koc (KOC)	152284	pH 1	(1) ACD
Koc (KOC)	152284	pH 4	(1) ACD
Koc (KOC)	152284	pH 7	(1) ACD
Koc (KOC)	152284	pH 8	(1) ACD
Koc (KOC)	152284	pH 10	(1) ACD
logD (LOGD)	7.00	pH 1	(1) ACD
logD (LOGD)	7.00	pH 4	(1) ACD
logD (LOGD)	7.00	pH 7	(1) ACD
logD (LOGD)	7.00	pH 8	(1) ACD
logD (LOGD)	7.00	pH 10	(1) ACD
logP (LOGP)	6.996+/-0.446		(1) ACD

Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	298.37		(1) ACD
Vapor Pressure (VP)	7.89E-06 Torr	25.0 deg C	(1) ACD

(1) Calculated using Advanced Chemistry Development (ACD) Software Solaris V4.76 ((C) 1994-2003 ACD)

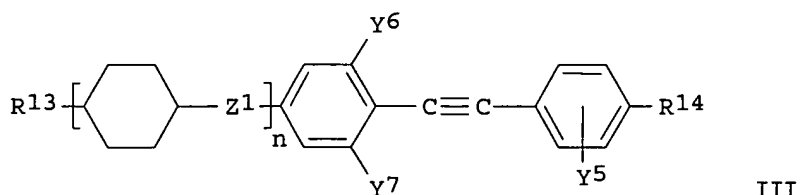
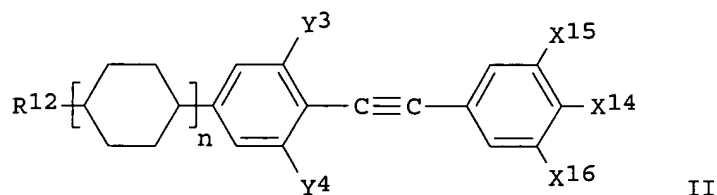
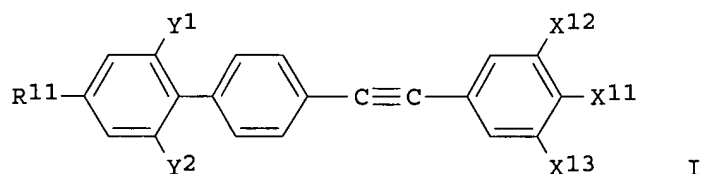
3 REFERENCES IN FILE CA (1962 TO DATE)
3 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1

AN 127:364222 CA
TI manufacture of liquid crystal device and liquid crystal display
IN Kuryama, Takeshi; Nakada, Hidetoshi; Ogawa, Hiroshi; Takeuchi, Kiyobumi; Fujisawa, Noburu
PA Dainippon Ink and Chemicals, Inc., Japan
SO Jpn. Kokai Tokkyo Koho, 24 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
IC ICM C09K019-42
ICS C09K019-18; C09K019-30; C09K019-54; G02F001-13
CC 74-13 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)
Section cross-reference(s): 75

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
	-----	---	-----	-----	-----
PI	JP 09255954	A2	19970930	JP 1997-6460	19970117
PRAI	JP 1996-7421		19960119		
GI					



AB The present invention relates to liq. crystal devices employing a novel polymer-dispersed liq. crystal compns. that contain the liq. crystals represented by I [R11 = C2-7 alkyl and alkoxy; X11 = F, Cl, F3CO, F3C, C1-5 alkyl, and alkoxy; X12, X13, Y1, and Y2 = independently H or F], II [R12 = C2-7 alkyl, alkenyl, and alkoxyalkyl; X14 = F, Cl, F3CO, F3C, C1-5 alkyl, and alkoxy; X15, X16, Y3, and Y4 = independently H or F; n = 0 or 1], and III [R13 = C2-7 alkyl or alkenyl; R14 = C1-7 alkyl, alkoxy, alkenyl and alkenyloxy; Y5 = H, F, and CH3; Y6 and Y7 = independently H or F; Z1 = single bond, COO, C2H4, and C4H8; n = 0 or 1] and alkylene di(meth)acrylate represented by H2C=CR41COO-R'-OCCCR42=CH2 [R41 and R42 = H or CH3; R' = C6-50 alkylene group, it may contain alicyclic group].

ST diacrylate polymer dispersed liq crystal device

IT Liquid crystal displays
Liquid crystals
(manuf. of liq. crystal device and liq. crystal display)

IT Acrylic polymers, preparation
RL: DEV (Device component use); PNU (Preparation, unclassified); PREP (Preparation); USES (Uses)
(manuf. of liq. crystal device and liq. crystal display)

IT 38444-13-2P 38690-77-6P 39969-28-3P 39969-29-4P 49763-64-6P
56131-49-8P 85583-83-1P 92118-81-5P 92118-82-6P 92118-83-7P
95480-29-8P 105895-14-5P 114834-78-5P 116903-47-0P 129738-34-7P
137198-91-5P 142256-81-3P 149705-67-9P 156243-60-6P 156243-62-8P
156243-63-9P 162142-85-0P 162142-86-1P 177572-85-9P 181885-66-5P
183436-87-5P 183436-88-6P 184161-94-2P 198279-53-7P 198279-54-8P
198279-55-9P 198279-57-1P 198336-24-2P 198559-55-6P 198586-69-5P
198586-70-8P
RL: DEV (Device component use); PNU (Preparation, unclassified); PREP (Preparation); USES (Uses)
(manuf. of liq. crystal device and liq. crystal display)

REFERENCE 2

AN 126:150603 CA

TI Nematic liquid crystal composition for active matrix liquid crystal display

IN Terajima, Kenji; Takeshita, Fusayuki; Yamamoto, Hitoshi; Kawayadota, Hiroaki

PA Chisso Corp, Japan

SO Jpn. Kokai Tokkyo Koho, 18 pp.
CODEN: JKXXAF

DT Patent

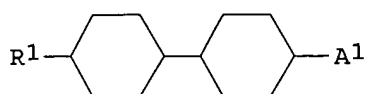
LA Japanese

IC ICM C09K019-46
ICS C09K019-30; G02F001-13

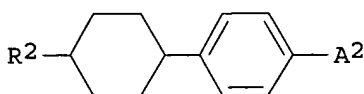
CC 74-13 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)

FAN.CNT 1

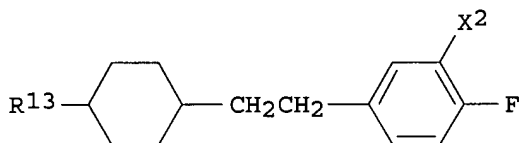
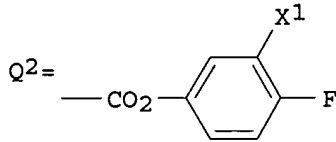
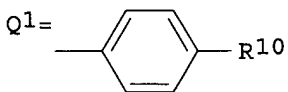
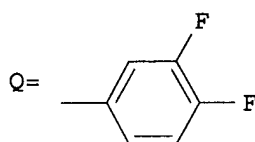
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
	-----	---	-----	-----	-----
PI	JP 08302353	A2	19961119	JP 1995-128995	19950428
PRAI	JP 1995-128995		19950428		
GI					



I



II



III

AB A liq. crystal compn. contg. (1) at least one first component selected from 4-(4-cyclohexylcyclohexyl)-1,2-difluorobenzene derivs. (I; R1 = C1-10 alkyl, C2-10 alkenyl; A1 = Q), (2) at least one second component selected from 4'-cyclohexyl-3,4-difluorobiphenyl derivs. (II; R2 = C1-10 alkyl, C2-10 alkenyl; A2 = Q), (3) at least one third component selected from cyclohexylbenzene derivs. II (R2, A2 = C1-10 alkyl, alkoxy, C2-10 alkenyl), cyclohexylcyclohexane derivs. I (R1, A1 = C1-10 alkyl, alkyl, C2-10 alkenyl), and 4-cyclohexylcyclohexanecarboxylate esters I (A1 = CO2R8; R1, R8 = C1-10 alkyl, C2-10 alkenyl), (4) at least one fourth component selected from 4-(4-cyclohexylcyclohexyl)benzene derivs. II (A2 = Q1; R2, R10 = C1-10 alkyl, C2-10 alkenyl) and (4-cyclohexylcyclohexyl)-1-fluorobenzene derivs. II (A2 = Q1, R10 = F; R2 = C1-10 alkyl, C2-10 alkenyl), (5) at least one fifth component selected from p-fluorophenyl 4-cyclohexylcyclohexanecarboxylate derivs. I (R1 = C1-10 alkyl, C2-10 alkenyl; A1 = Q2, X1 = H or F), and (6) at least one sixth component selected from 4-(2-cyclohexylethyl)-1-fluorobenzene (III; R13 = C1-10 alkyl, C2-10 alkenyl; X2 = H, F), is claimed. A liq. crystal device using above compn. is claimed. This liq. crystal compn. shows nematic phase at a broad temp. range, low viscosity, and high specific resistance and provides an active matrix liq. crystal display with high contrast, high speed response, and high reliability.

ST nematic liq crystal compn; active matrix liq crystal display; cyclohexylcyclohexyldifluorobenzene nematic liq crystal compn; cyclohexyldifluorobiphenyl nematic liq crystal compn; cyclohexylbenzene nematic liq crystal compn; cyclohexylcyclohexane nematic liq crystal compn; cyclohexylcyclohexanecarboxylate nematic liq crystal compn; cyclohexylcyclohexylbenzene nematic liq crystal compn; cyclohexylcyclohexylfluorobenzene nematic liq crystal compn; cyclohexylethylfluorobenzene nematic liq crystal compn; fluorophenyl cyclohexylcyclohexanecarboxylate nematic liq crystal compn

IT Liquid crystal displays
(nematic liq. crystal compn. for active matrix liq. crystal display)

IT Liquid crystals
(nematic; nematic liq. crystal compn. for active matrix liq. crystal display)

IT	79709-84-5	79912-83-7	79912-85-9	80944-44-1	81701-13-5
	82832-27-7	82832-57-3	82985-79-3	82985-80-6	84656-75-7
	84656-77-9	85312-59-0	86504-59-8	88038-92-0	88416-69-7
	88878-50-6	94840-77-4	96624-52-1	107215-73-6	118164-50-4
	118164-51-5	119990-81-7	129738-34-7	129738-42-7	134412-17-2
	134412-18-3	142256-81-3	142400-92-8	186448-44-2	186448-45-3
	186448-46-4				

RL: TEM (Technical or engineered material use); USES (Uses)
(component for liq. crystal compn.; nematic liq. crystal compn. for active matrix liq. crystal display)

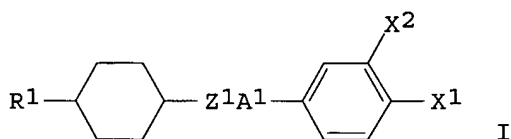
REFERENCE 3

AN 117:59084 CA
 TI Halogenated alkenyl compounds, liquid-crystal mixtures containing them, and their use for electrooptical purposes
 IN Buchecker, Richard; Germann, Alfred; Schadt, Martin; Vilinger, Alois
 PA Hoffmann-La Roche, F., und Co. A.-G., Switz.
 SO Eur. Pat. Appl., 25 pp.
 CODEN: EPXXDW
 DT Patent
 LA German
 IC ICM C09K019-34
 ICS C09K019-30; C07C025-24; C07D239-26; C07D213-26; G02F001-1337
 CC 74-13 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)
 Section cross-reference(s): 75

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 475273	A1	19920318	EP 1991-114986	19910905
	EP 475273	B1	19990407		
	R: CH, DE, FR, GB, IT, LI, NL				
	US 5292452	A	19940308	US 1991-747033	19910819
	JP 07010787	A2	19950113	JP 1991-261260	19910913
	JP 3035392	B2	20000424		
PRAI	CH 1990-2992		19900914		
	CH 1991-1434		19910514		

GI



AB The compds. have the general formula I, where Z1 = single bond or CH2CH2; A1 = 1,4-phenylene, pyrimidin-2,5-diyl, pyridin-2,5-diyl, or (when Z1 = CH2CH2) trans-1,4-cyclohexylene; X1 = F or Cl, X2 = F, Cl, or H; and R1 = C2-12 trans-1-alkenyl.

ST halogenated alkenyl compd liq crystal mixt

IT Liquid crystals

(mixts., contg. halogenated alkenyl compds.)

IT Optical imaging devices

(electro-, liq.-crystal, mixts. for, contg. halogenated alkenyl compds.)

IT	142275-91-0	142275-93-2	142275-95-4	142275-96-5	142393-69-9
	142393-70-2	142393-71-3	142393-72-4	142393-73-5	142393-74-6
	142394-66-9				

RL: TEM (Technical or engineered material use); USES (Uses)

(liq. crystal, for display devices)

IT	105640-07-1P	124500-61-4P	132951-11-2P	142256-87-9P	142256-88-0P
	142256-89-1P	142256-90-4P	142256-91-5P	142256-92-6P	142256-93-7P
	142256-94-8P	142256-95-9P	142256-96-0P	142256-97-1P	142256-98-2P
	142256-99-3P	142257-00-9P	142257-01-0P	142257-02-1P	142257-03-2P
	142257-04-3P	142257-05-4P	142257-06-5P	142257-07-6P	142257-08-7P
	142257-09-8P	142257-10-1P	142257-11-2P	142257-12-3P	142257-13-4P
	142257-14-5P	142279-97-8P			

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. and reaction of, in formation of compds. for liq.-crystal mixts. and display devices)

IT	142256-69-7P	142256-70-0P	142256-71-1P	142256-72-2P	142256-73-3P
	142256-74-4P	142256-75-5P	142256-76-6P	142256-77-7P	142256-78-8P
	142256-79-9P	142256-80-2P	142256-81-3P	142256-82-4P	142256-83-5P
	142256-84-6P	142256-85-7P	142256-86-8P		

RL: PREP (Preparation)

(prepn. of, for liq.-crystal mixts. and display devices)